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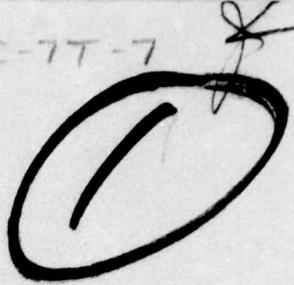
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ON THE DISTRIBUTION OF SOME STOCHASTIC COMPARTMENTAL MODELS
HAVING TIME-DEPENDENT TRANSITION PROBABILITIES, WITH
APPLICATIONS TO RELIABILITY

A Dissertation

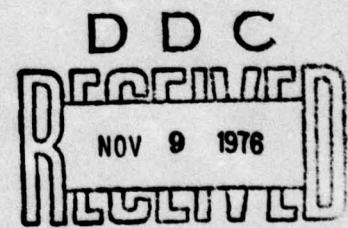
by

JON OHMAN EPPERSON

Submitted to the Graduate College of
Texas A&M University
in partial fulfillment of the requirement for the degree of

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August 1976



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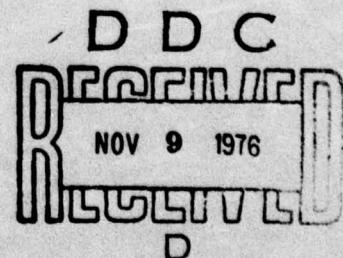
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ABSTRACT

On the Distribution of Some Stochastic Compartmental Models
having Time-Dependent Transition Probabilities, with
Applications to Reliability. (August 1976)

Jon O. Epperson, B.S., University of New Mexico;
M.A., University of Missouri

Chairman of Advisory Committee: Dr. J.H. Matis

The cumulant generating functions of some multi-compartment stochastic models having time-dependent transition rates are derived. Using these, the first and second moments of the stochastic distributions are found. Under certain assumptions concerning the initial conditions the stochastic distributions are specifically identified. The models investigated are the n-compartment mixed catenary-mammillary model and the n-compartment general irreversible model. These derivations are then used to analyze some reliability systems. In particular, the catenary portion of the mixed model is used to obtain stochastic analyses of a standby redundant system. The mixed model is used for a system wherein a component is subject to competing-risks with standby components. The general model is employed to evaluate a mission reliability with a hierarchical failure structure.



to the memory of my father

Mitchell S. Epperson

he dedicated his life to helping people

ACKNOWLEDGEMENTS

Dr. J. H. Matis was encouraging, optimistic and creative. Whatever the probability densities are for these human attributes, I believe he is beyond the $+3\sigma$ point on each. This made me particularly fortunate to have had him for my advisor.

I wish to thank the other members of my committee, Dr. J. G. H. Thompson, Dr. H. O. Hartley, Dr. L. J. Ringer and Dr. P. W. Smith for their time and willingness to work with me. I am honored to have had members of such distinction.

I am especially grateful to my wife Susan, and my children, Mark and Elaine for their patience and sacrifice. While I had essentially one major day-to-day concern, school, Susan coped with the myriad details of raising a young family and keeping the household on course. With all of this she still found time to type this manuscript. My thanks to her will be a continuing process.

I feel deeply grateful for my parents' example of hard work and perseverance. They instilled in all their children a desire for learning. My parents-in-law, Mrs. Lois A. Smith and the late Dr. T. L. Smith, by their achievements and lifelong work in higher education, also inspired me to seek this degree.

Finally I wish to thank the U. S. Air Force and the American taxpayers for providing me and my family with a financial security enjoyed by few graduate students.

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1. INTRODUCTION

1.1 Preliminaries

Compartmental analysis is a relatively new branch of mathematical modeling which has undergone considerable growth in recent years. Contributions to this theory have come from diverse scientific disciplines which attests to the generality and wide applicability of the method. In the general compartmental modeling problem, one wishes to describe the movement of a substance through a system. This may, for example, be the movement of a chemical through an organism, a person through an organization or perhaps an organism through an ecosystem. Whatever the situation, it is assumed the system under consideration can be divided into homogeneous compartments. The rate at which the substance leaves a compartment is usually assumed to be proportional to the amount of substance in that compartment. Other mathematical formulations for compartmental transitions have been investigated and are summarized in Section 1.3. Thinking in terms of a unit or particle of this substance, it is further assumed that one unit in a compartment acts independently of every other unit in that compartment.

It is clear these assumptions greatly restrict the problems which can be modeled in this way. However the class of problems which fits these assumptions is still quite broad. Sheppard [1962], Rescigno and Segre [1965], Atkins [1969] and Jacquez [1972] discuss a

Citations will follow the format of Biometrics.

wide variety of such problems.

In classical compartmental analysis the transitions from one compartment to another are assumed to be deterministic in nature. This assumption leads to a system of linear, first-order differential equations whose solution yields the amount of substance in a given compartment at any time. Many systems have been adequately modeled in this way. However, in some cases more realism can be put into the model by assuming a stochastic or probabilistic behavior for the compartmental transitions. Matis [1970] states this advantage of the probabilistic approach in the following way;

...a compartmental model can only claim to represent an 'approximate' theoretical background for the biological observed phenomena, in that it employs an abstraction of 'transfer' of particles without specifying a detailed causative theory responsible for the transfer mechanisms. It is also because of this approximate feature that a stochastic compartmental theory is more realistic in that a detailed causative mechanism which is lacking in the deterministic model is replaced by a stochastic model.

The stochastic model not only has this added realism but in some cases one can recover the deterministic model in that the expectation of the stochastic model is the same as the deterministic solution. Such a circumstance is discussed in Matis [1970]. This is not to say stochastic modeling will or should replace deterministic modeling. Matis [1976] argues that while some problems are adequately modeled deterministically, other problems currently approached deterministically could be modeled better stochastically.

Uppuluri and Bernard [1967] and Grandijan and Bergner [1972] discuss stochastic models whose expectations are not the same as their corresponding deterministic models.

1.2 Applications

In this section examples will be presented to illustrate the variety of problems to which the compartmental technique has been applied. These examples are divided into deterministic models and stochastic models. It is convenient to illustrate a compartmental model using a schematic wherein boxes represent compartments and arrows represent intercompartmental transitions. The transition rate from compartment j to compartment i is denoted λ_{ij} .

1.2.1 Applications using Deterministic Models

Atkins [1969] gives a comprehensive account of the use of deterministic methods in biological systems. One of his examples (p. 69) is the two-compartment model depicted in Figure 1. This was used to model the movement of water within a rabbit. Here the primary question is not how much water is in each compartment but rather the kinetics of the

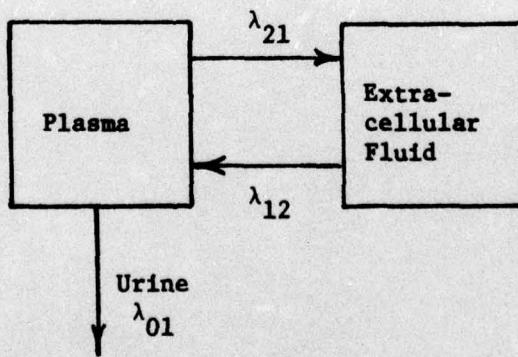


Figure 1

Two-Compartment Model for Water Movement Within a Rabbit

water within the system. To do this the water must be labeled and the movement of the labeled substance, called tracer, is observed.

In this study inulin was used as a tracer substance. A single intravenous injection of inulin was given and the concentration of inulin within the plasma determined at subsequent time periods. These data then allowed for an estimation of the exchange rates (λ_{12} and λ_{21}) of water between the plasma and extracellular fluid and the rate of excretion of water as urine (λ_{01}).

This example is typical of a situation which often occurs. That is, one compartment, the plasma, is readily accessible to the researcher whereas the other compartment, the extracellular fluid, is not so accessible. The compartmental approach often allows estimates to be made on regions of a system where observations cannot be made directly.

The compartmental approach was used by Herbst [1963] to model organizational commitment. He assumed the decision structure shown in Figure 2. Using time series data on the departures of individuals from firms, he was able to estimate the transition rates (λ_{ij}) as well as the number of persons in each compartment at time t. Note that this example also includes compartments not readily observable but whose content is invaluable to a firm's personnel recruitment planning. This is an example in which the deterministic approach provided an excellent fit of the data.

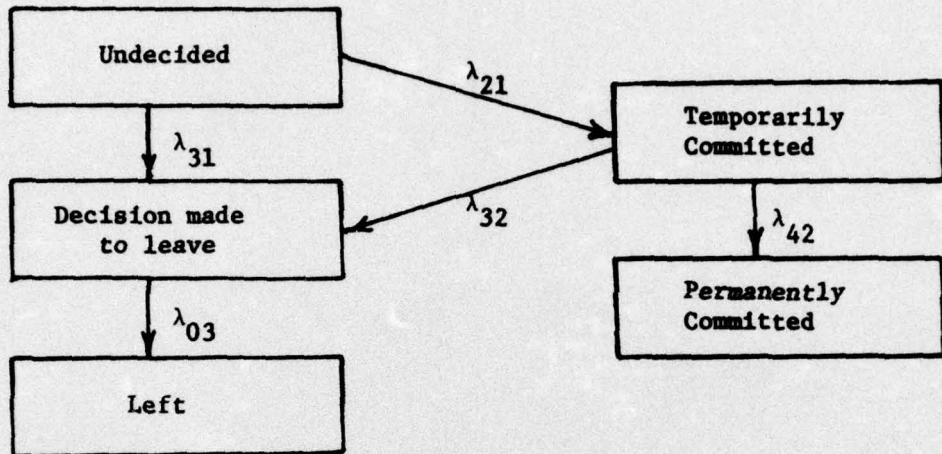


Figure 2

Organizational Commitment Model as a Compartmental System

1.2.2 Applications using Stochastic Models

Using indigestible, plastic beads as tracers, Matis [1970] was able to estimate the parameters for the ruminant gastrointestinal tract illustrated in Figure 3. (In addition he evaluated the fit of this model and found a two-compartment model to be superior.)

At time $t = 0$, 4,000 of the beads were placed into a sheep's rumen. The feces were collected at fixed time intervals and bead counts made. Using these time series data the transition rates were estimated by a method which made use of the stochastic compartmental distribution and the serial correlation of the data.

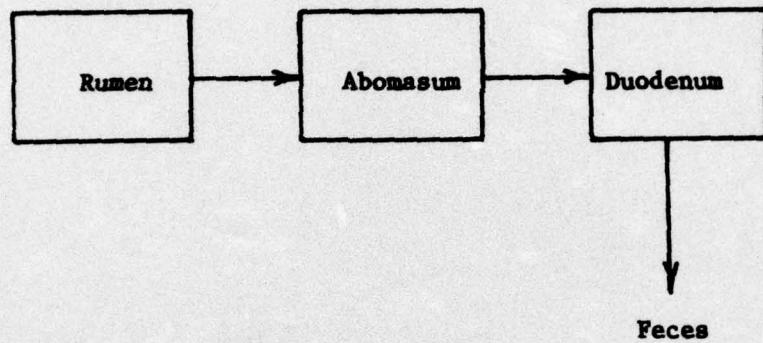


Figure 3

Ruminant Gastrointestinal Tract as a Compartmental Model

For a final example of the use of stochastic compartmental modeling, consider the compartmental arrangement of Figure 4. This is known as a mammillary model and has an abundance of applications. Matis et al. [1974] consider the central compartment to be the blood stream and the peripheral compartments to be tissue groups. A particle in the blood stream can pass to one of the k tissue groups with rate α or leave the system completely with rate β . Once a particle has entered a tissue group it can leave the system with rate γ .

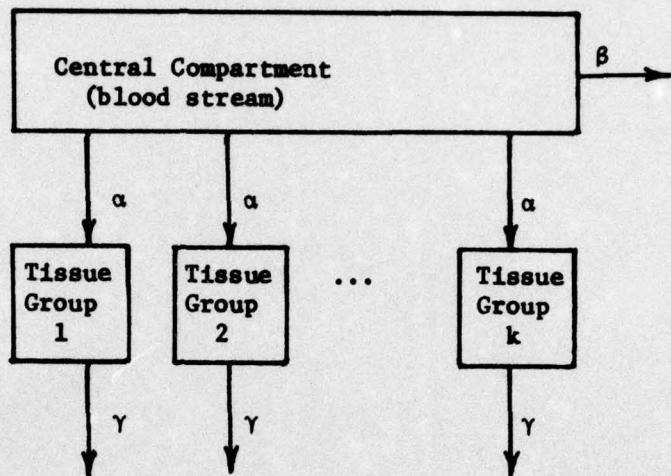


Figure 4

A Mammillary Compartmental Model with k Peripheral Compartments

Using stochastic theory they determine lower bounds on the probability of having a given number of particles present in a given tissue group. This application has implications in cancer research under the assumption that a carcinogen present in the blood stream induces cancer in a tissue group if a critical threshold level of the substance is reached in that tissue group. This solution requires the use of the stochastic theory and cannot be solved with the deterministic model alone.

1.3 Literature Review

This dissertation is primarily concerned with the derivation of some particular stochastic models and their applications. The deterministic counterparts to these models will play a role in the applications but are derived by distribution theoretic considerations rather than methods found in the literature of deterministic compartmental analysis. This literature is of interest here due to its place in the evolution of the compartmental theory.

Atkins [1969] was previously referenced for his account of deterministic methods in biological systems. Other references for the deterministic method are Sheppard [1962], Rescigno and Segre [1965] and Jacquez [1972].

Bartholomay [1958] was one of the first to suggest the stochastic approach and solved the one-compartment model. Since the initial work of Bartholomay, the theoretical evolution of stochastic compartmental analysis has proceeded in two general categories. On the one hand generalizations have been made to the mathematical formulation of the transition rates and on the other hand modifications and extensions have been made to the compartmental structure itself.

Initially, transition rates were taken to be constants. These have since been modified in a number of independent ways. Uppuluri and Bernard [1967] introduce the idea of a random component between compartments and Chiang [1968] incorporates time-dependent input rates. A two-compartment system having all transition rates time-dependent is solved by Puri [1968]. However, his solution involves a series

representation for the probability generating function. Concentration-dependent transition rates are introduced by Bellman [1970]. Sykes [1969] and Soong [1971, 1972] treat the transition rates as random variables.

The one-compartment model is generalized by Thakur [1972] such that the compartmental input is time-dependent and in addition, the usual assumption that the initial number of particles be known is dropped. Instead the more general assumption is made that their distribution is known. One generalization which has received less attention than those applied to the transition rates is the introduction of age-dependency to compartments. Blaxter's [1956] model for passage of particles through the gastrointestinal tract of ruminants is generalized by Matis [1972] to include gamma age-dependency in the first compartment. Purdue [1974] investigates one and two-compartment models in which particles present at time zero have different lifetime distributions from those arriving later. A queuing theoretic approach is used in this analysis.

Results which are advancements in compartmental structure of course begin with the solutions to the one and two-compartment systems which assume constant transition rates. Matis and Carter [1969] find the first and second moments of the two-compartment system. Matis and Hartley [1971] solve the general n-compartment model with constant transition rates and propose a method for estimating the parameters based on Hartley's [1961] modified Gauss-Newton method for fitting non-linear regression functions by least squares. In this model a particle in one compartment can transfer to any other compartment. Hence the

flow is completely reversible. Cardenas and Matis [1974] solve the irreversible n-compartment catenary system and the irreversible n-compartment mammillary system assuming time-dependent input, output and transition rates. These results are in turn used in Cardenas and Matis [1975] to solve the general reversible two-compartment model with time-dependent input, output and transition rates. A special class of n-compartment systems is investigated by Cardenas and Matis [1975] wherein the structure is general and reversible but the transition rates are some multiple of a time-dependent function.

Matis [1976] presents an overview of deterministic and stochastic techniques. In doing so he discusses three general steps in applying the compartmental method to specific systems. The first step is the development of a plausible and relevant compartmental model for the system of interest. The second step is the derivation of the mathematical solution to the proposed model and the final step consists of obtaining the optimal statistical design for data acquisition and then estimating the parameters of the model from these data.

The estimation phase is by far the most difficult and the least developed of these three steps. See Kodell [1974] for a comprehensive review of estimation procedures in stochastic modeling.

1.4 Assumptions and Notation

Let $X_i(t)$ denote a stochastic variable indicating the number of units in the i^{th} compartment of a system at time t . The system will consist of a fixed number of compartments, n , and compartment zero will

indicate the system exterior. The transition rate from the j^{th} compartment to the i^{th} compartment at time t will be denoted $\lambda_{ij}(t)$. The change in the number of units in compartment i during the time interval $(t, t+\Delta t)$ is $\Delta X_i(t)$, i.e.,

$$\Delta X_i(t) = X_i(t+\Delta t) - X_i(t)$$

for $i = 1, 2, \dots, n$.

It is assumed units transfer in any of three ways; a unit may enter a compartment from the system exterior, move from one compartment to another compartment or exit a compartment to the exterior of the system. These transfers have various names depending on the discipline. For example, the ecologist would speak of these as immigration, migration and death, or the biologist as ingestion, circulation and excretion. The probability of these three events occurring will now be defined as follows:

Prob {a single unit enters compartment j

from outside the system in the interval

$(t, t+\Delta t)$ } =

$$\lambda_{j0}(t)\Delta t + o(\Delta t) \quad j = 1, 2, \dots, n,$$

Prob {a single unit in compartment j moves to

compartment i in the interval $(t, t+\Delta t)$ } =

$$X_j(t)\lambda_{ij}(t)\Delta t + o(\Delta t) \text{ for all } i \text{ and } j,$$

and

$$\begin{aligned} \text{Prob } \{ \text{a single unit in compartment } j \text{ leaves the} \\ \text{system in the interval } (t, t+\Delta t) \} = \\ x_j(t)\lambda_{0j}(t)\Delta t + o(\Delta t) \quad \text{for all } j. \end{aligned}$$

Note that the probability of two or more events occurring during the interval $(t, t+\Delta t)$ is $o(\Delta t)$.

The following assumptions are made throughout the dissertation:

- i) The units in a compartmental system act independent of each other.
- ii) Units entering the system from the outside do not alter the system's behavior.
- iii) The initial probability distribution of units within the compartments is known and in particular the cumulant generating function of this distribution is denoted $k(\theta_1, \theta_2, \dots, \theta_n)$.

1.5 Overview

In Cardenas and Matis [1974], the stochastic solution to the n-compartment catenary and mammillary models with irreversible, time-dependent transition probabilities is solved. The schematic illustrating the catenary model is shown in Figure 5.

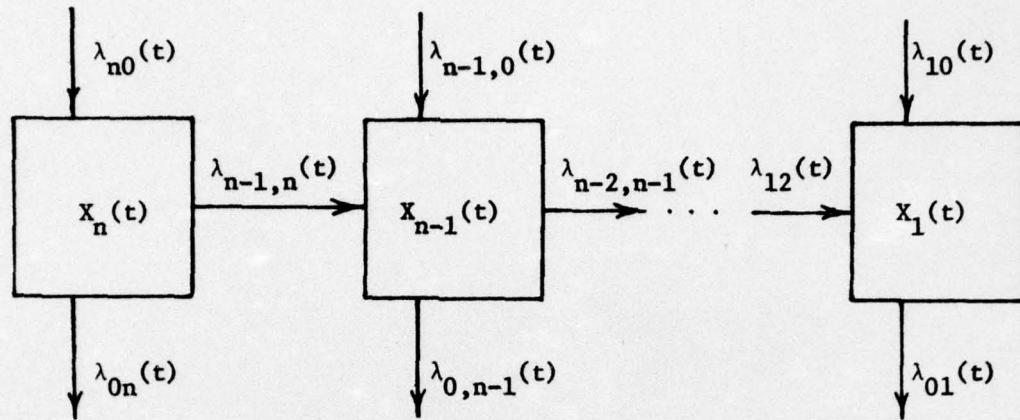


Figure 5

n-Compartment, Irreversible Catenary System

The joint cumulant generating function of the stochastic vector $(X_1(t), X_2(t), \dots, X_n(t))$ is found in terms of the cumulant generating function for the initial distribution, $k(\theta_1, \theta_2, \dots, \theta_n)$. When the initial number of units is assumed to be $X_i(0) = x_i$, $i = 1, 2, \dots, n$, the form of this generating function is shown by Matis [1970] to correspond to a sum of multinomials and Poissons.

In a similar manner, the joint cumulant generating function associated with the mammillary model illustrated in Figure 6 is derived in Cardenas and Matis [1974].

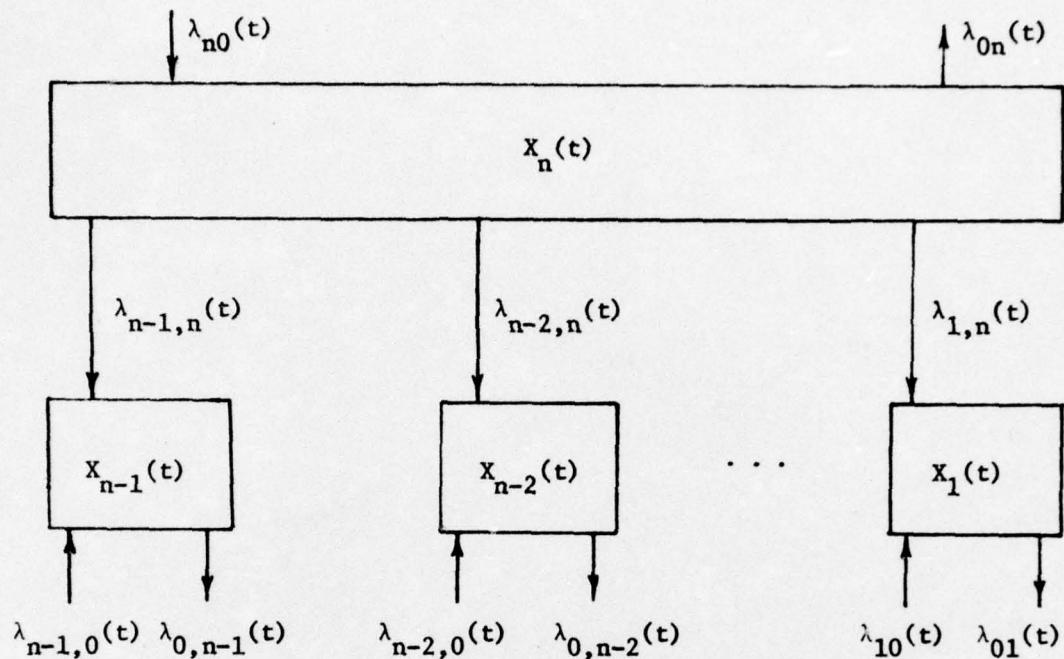


Figure 6

n-Compartment, Irreversible Mammillary System

These two systems are combined and the resulting mixed model is derived in Section 2 of the present study. Using the cumulant generating function, the expectation and variance for each compartment as well as the covariance between any two compartments are found as a function of time.

This model is generalized further in Section 3 to a completely general irreversible model in which a unit in compartment n can transfer to any of the $n-1$ remaining compartments and a unit in the $(n-1)^{st}$ compartment can transfer to any of the $n-2$ other compartments, etc. As in Section 2, the cumulant generating function and the first and second moments of the stochastic distribution are derived.

Section 4 contains applications to reliability analyses using a compartmental approach. Systems of components in various redundant configurations are considered and standard properties such as the system reliability, the mean time to system failure and the variance of the lifelength are derived as functions of the transition rates.

Other areas of research and possible applications in compartmental analysis are discussed in Section 5.

2. THE MIXED MODEL

In this section a compartmental model is considered which is a mixture of the catenary model and mammillary model discussed in Section 1.5. The form of this mixed model is illustrated in Figure 7. The stochastic variable $X_i(t)$ indicates the number of units in the i^{th} compartment at time t . The transition rates $\lambda_{ij}(t)$ are the intensity coefficients for a unit moving from compartment j to compartment i at time t .

The exact multivariate distribution for the stochastic vector $(X_1(t), X_2(t), \dots, X_n(t))$ will be determined. The method employed in this derivation was first used for time-dependent compartmental models by Cardenas and Matis [1974] in solving the n -compartment catenary and mammillary models previously discussed.

The technique consists of first finding a partial differential equation for a generating function of the distribution. This partial differential equation is then solved and the multivariate distribution is identified by appealing to the unique form of the generating function.

One method for finding the desired partial differential equation is to find the Kolmogorov forward equation associated with this model's single event probabilities. From the forward equation the partial differential equation follows easily. This method is intuitively appealing. Essentially, one starts with the definition of a partial derivative and proceeds to the partial differential equation. However, this approach is tedious and a much more elegant technique was devised by

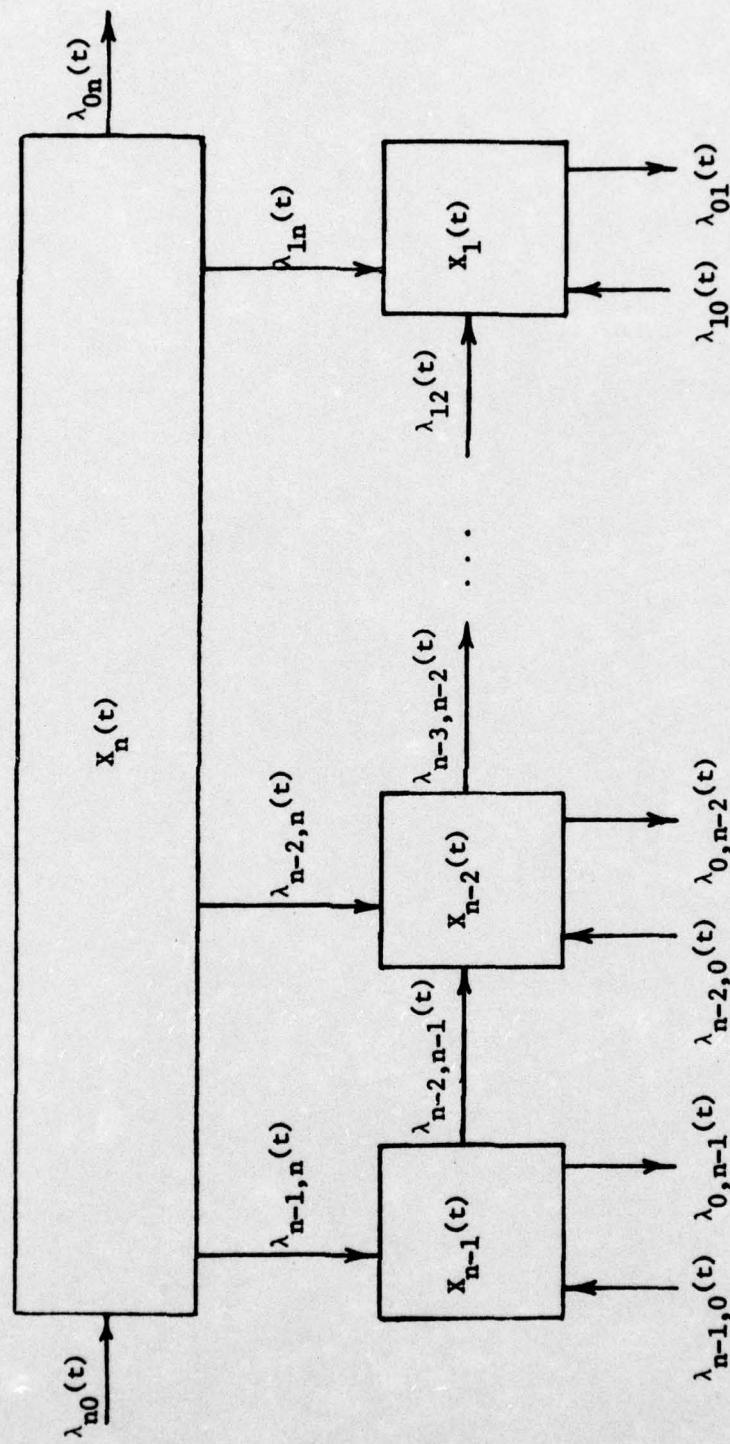


Figure 7
The n -Compartment Mixed Catenary-Mammillary Model

Bartlett [1949], which allows one to write down the partial differential equation with relative ease. A description of this "random variable" technique can also be found in Bailey [1964].

2.1 Three-Compartment Mixed Model

To illustrate the solution to the mixed model, the three-compartment model depicted in Figure 8 will first be solved in detail. Then the solution for the n-compartment mixed model will be sketched following analogous steps.

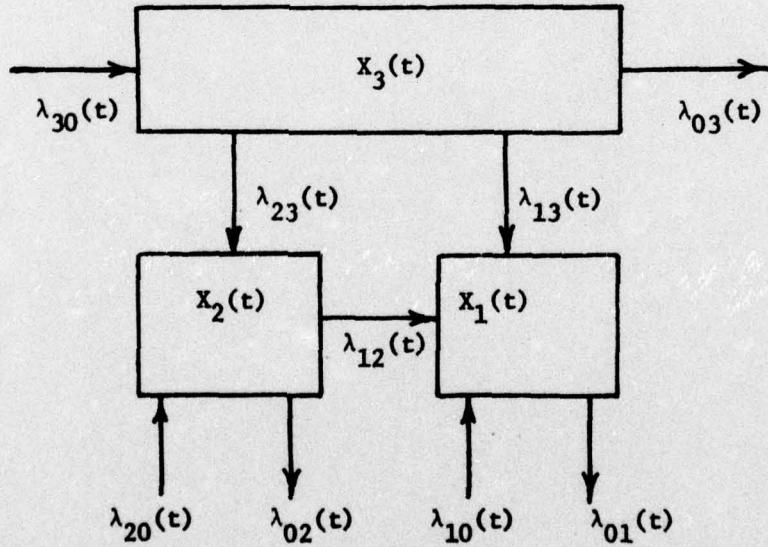


Figure 8
Three-Compartment Mixed Catenary-Mammillary Model

2.1.1 The Partial Differential Equation for the Cumulant Generating Function

All of the possible transition probabilities can be summarized as follows:

Prob {a single unit enters compartment i from outside the system in the interval $(t, t+\Delta t)$ } =
 $\lambda_{10}(t)\Delta t + o(\Delta t)$ for $i = 1, 2, 3.$

Prob {a single unit moves from compartment j to compartment i in the interval $(t, t+\Delta t)$ } =
 $x_j(t)\lambda_{ij}(t)\Delta t + o(\Delta t)$ for $j = 1, 2, 3, i = 0, 1, 2, 3.$

There are nine events with probability of first order magnitude of Δt . All other events can be ignored because their probability is $o(\Delta t)$. These nine events imply:

$$\begin{aligned} \text{Prob } & \{\Delta X_1(t) = k_1, \Delta X_2(t) = k_2, \Delta X_3(t) = k_3 | \\ & x_1(t), x_2(t), x_3(t)\} = \\ & \left\{ \begin{array}{ll} x_3(t)\lambda_{13}(t)\Delta t + o(\Delta t) & k_3=-1, k_1=+1 \text{ } i=1,2. \\ x_j(t)\lambda_{0j}(t)\Delta t + o(\Delta t) & k_j=-1, j=1,2,3, \text{ all other } k's \\ & \text{are zero.} \\ x_2(t)\lambda_{12}(t)\Delta t + o(\Delta t) & k_2=-1, k_1=+1 \text{ all other } k's \\ & \text{are zero.} \\ \lambda_{j0}(t)\Delta t + o(\Delta t) & k_j=+1, j=1,2,3, \text{ all other } k's \\ & \text{are zero.} \end{array} \right. \end{aligned}$$

where $\Delta X_i(t) = x_i(t+\Delta t) - x_i(t)$ for all i.

Now applying Bartlett's "random variable" technique one obtains the partial differential equation

$$\begin{aligned}
 \frac{\partial M(\theta_1, \theta_2, \theta_3, t)}{\partial t} = & \sum_{i=1}^2 (e^{-\theta_3 + \theta_{i-1}}) \lambda_{i3}(t) \frac{\partial M(\theta_1, \theta_2, \theta_3, t)}{\partial \theta_3} \\
 & + \sum_{j=1}^3 (e^{-\theta_j - 1}) \lambda_{0j}(t) \frac{\partial M(\theta_1, \theta_2, \theta_3, t)}{\partial \theta_j} \\
 & + (e^{-\theta_2 + \theta_{1-1}}) \lambda_{12}(t) \frac{\partial M(\theta_1, \theta_2, \theta_3, t)}{\partial \theta_2} \\
 & + \sum_{j=1}^3 (e^{-\theta_j - 1}) \lambda_{j0}(t) M(\theta_1, \theta_2, \theta_3, t)
 \end{aligned} \tag{1}$$

for the joint moment generating function of $X_1(t)$, $X_2(t)$ and $X_3(t)$.

After dividing (1) by $M(\theta_1, \theta_2, \theta_3, t)$ and rearranging terms, the differential equation for the cumulant generating function $K(\theta_1, \theta_2, \theta_3, t)$ is found to be

$$\begin{aligned}
 \frac{\partial K(\theta_1, \theta_2, \theta_3, t)}{\partial t} = & (e^{-\theta_{1-1}}) \lambda_{01}(t) \frac{\partial K(\theta_1, \theta_2, \theta_3, t)}{\partial \theta_1} \\
 & + \left[(e^{-\theta_{2-1}}) \lambda_{02}(t) + (e^{-\theta_2 + \theta_{1-1}}) \lambda_{12}(t) \right] \frac{\partial K(\theta_1, \theta_2, \theta_3, t)}{\partial \theta_2}
 \end{aligned}$$

$$\begin{aligned}
 & + \left[(e^{-\theta_3})_{-1} \lambda_{03}(t) + \sum_{i=1}^2 (e^{-\theta_3+\theta_i})_{-1} \lambda_{i3}(t) \right] \frac{\partial K(\theta_1, \theta_2, \theta_3, t)}{\partial \theta_3} \\
 & + \sum_{j=1}^3 (e^{\theta_j})_{-1} \lambda_{j0}(t). \tag{2}
 \end{aligned}$$

2.1.2 The Joint Cumulant Generating Function

Equation (2) is a quasi-linear partial differential equation which can be solved using characteristic theory (see Ford [1955] or Garabedian [1964]). The characteristic equations associated with (2) are determined by the system of ordinary differential equations

$$\begin{aligned}
 \frac{dt}{1} = \frac{d\theta_1}{(1-e^{-\theta_1}) \lambda_{01}(t)} = \frac{d\theta_2}{(1-e^{-\theta_2}) \lambda_{02}(t) + (1-e^{\theta_2+\theta_1}) \lambda_{12}(t)} = \\
 \frac{d\theta_3}{(1-e^{-\theta_3}) \lambda_{03}(t) + \sum_{i=1}^2 (1-e^{-\theta_3+\theta_i}) \lambda_{i3}(t)} = \\
 \frac{dK(\theta_1, \theta_2, \theta_3, t)}{\sum_{j=1}^3 (e^{\theta_j})_{-1} \lambda_{j0}(t)}. \tag{3}
 \end{aligned}$$

Letting $v_1 = (e^{\theta_1} - 1)$, and hence $dv_1 = e^{\theta_1} d\theta_1$, these subsidiary equations can be rewritten as

$$\begin{aligned} dv_1 &= v_1 \lambda_{01}(t) dt, \\ dv_2 &= [(v_2 - v_1) \lambda_{12}(t) + v_2 \lambda_{02}(t)] dt, \\ dv_3 &= [(v_3 - v_2) \lambda_{23}(t) + (v_3 - v_1) \lambda_{13}(t) + v_3 \lambda_{03}(t)] dt, \\ dK(\theta_1, \theta_2, \theta_3, t) &= \left[\sum_{j=1}^3 v_j \lambda_{j0}(t) \right] dt. \end{aligned} \quad (4)$$

This system of differential equations can be solved sequentially, obtaining,

$$\begin{aligned} v_1 &= c_1 \exp \left\{ \int_0^t \lambda_{01}(z) dz \right\}, \\ v_2 &= c_2 \exp \left\{ \int_0^t [\lambda_{12}(z) + \lambda_{02}(z)] dz \right\} \\ &\quad - c_1 \int_0^t \lambda_{12}(t_1) \exp \left\{ \int_0^{t_1} \lambda_{01}(z) dz + \int_{t_1}^t [\lambda_{12}(z) + \lambda_{02}(z)] dz \right\} dt_1, \\ v_3 &= c_3 \exp \left\{ \int_0^t [\lambda_{23}(z) + \lambda_{13}(z) + \lambda_{03}(z)] dz \right\} \\ &\quad - c_2 \int_0^t \lambda_{23}(t_2) \exp \left\{ \int_0^{t_2} [\lambda_{12}(z) + \lambda_{02}(z)] dz + \int_{t_2}^t [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz \right\} dt_2 \end{aligned}$$

$$\begin{aligned}
& - c_1 \left[\int_0^t \lambda_{13}(t_2) \exp \left\{ \int_0^{t_2} \lambda_{01}(z) dz + \int_{t_2}^t [\lambda_{23}(z) + \lambda_{13}(z) + \lambda_{03}(z)] dz \right\} dt_2 \right. \\
& - \int_0^t \int_0^{t_2} \lambda_{12}(t_1) \lambda_{23}(t_2) \exp \left\{ \int_0^{t_1} \lambda_{01}(z) dz + \int_{t_1}^{t_2} [\lambda_{12}(z) + \lambda_{02}(z)] dz \right. \\
& \left. \left. + \int_{t_2}^t [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz \right\} dt_1 dt_2 \right]
\end{aligned}$$

and

$$\begin{aligned}
K(\theta_1, \theta_2, \theta_3, t) = & c_4 + c_3 \int_0^t \lambda_{30}(t_3) \exp \left\{ \int_0^{t_3} [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz \right\} dt_3 \\
& + c_2 \left[\int_0^t \lambda_{20}(t_3) \exp \left\{ \int_0^{t_3} [\lambda_{12}(z) + \lambda_{02}(z)] dz \right\} dt_3 \right. \\
& - \int_0^t \int_0^{t_3} \lambda_{30}(t_3) \lambda_{23}(t_2) \exp \left\{ \int_0^{t_2} [\lambda_{12}(z) + \lambda_{02}(z)] dz \right. \\
& \left. \left. + \int_{t_2}^{t_3} [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz \right\} dt_2 dt_3 \right] \\
& + c_1 \left[\int_0^t \lambda_{10}(t_3) \exp \left\{ \int_0^{t_3} \lambda_{01}(z) dz \right\} dt_3 \right. \\
& - \int_0^t \int_0^{t_3} \lambda_{20}(t_3) \lambda_{12}(t_1) \exp \left\{ \int_0^{t_1} \lambda_{01}(z) dz \right. \\
& \left. \left. + \int_{t_1}^{t_3} [\lambda_{12}(z) + \lambda_{02}(z)] dz \right\} dt_1 dt_3 \right] \\
& - \int_0^t \int_0^{t_3} \lambda_{30}(t_3) \lambda_{13}(t_2) \exp \left\{ \int_0^{t_2} [\lambda_{12}(z) + \lambda_{02}(z)] dz \right.
\end{aligned}$$

$$\begin{aligned}
& + \int_{t_2}^{t_3} [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz \Big\} dt_2 dt_3 \\
& + \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} \lambda_{30}(t_3) \lambda_{12}(t_1) \lambda_{23}(t_2) \exp \left\{ \int_0^{t_1} \lambda_{01}(z) dz \right. \\
& \left. + \int_{t_1}^{t_2} [\lambda_{12}(z) + \lambda_{02}(z)] dz + \int_{t_2}^{t_3} [\lambda_{13}(z) + \lambda_{23}(z) \right. \\
& \left. + \lambda_{03}(z)] dz \right\} dt_1 dt_2 dt_3. \tag{5}
\end{aligned}$$

Now again working sequentially with (5) and substituting back the values of V_1 , V_2 and V_3 one can solve for the arbitrary constants c_1 , c_2 , c_3 and c_4 . This results in

$$\begin{aligned}
c_1 &= u_1(\theta_1, \theta_2, \theta_3, t) = (e^{\theta_1} - 1)p_{11}(t), \\
c_2 &= u_2(\theta_1, \theta_2, \theta_3, t) = (e^{\theta_1} - 1)p_{12}(t) + (e^{\theta_2} - 1)p_{22}(t), \\
c_3 &= u_3(\theta_1, \theta_2, \theta_3, t) = (e^{\theta_1} - 1)p_{13}(t) + (e^{\theta_2} - 1)p_{23}(t) + (e^{\theta_3} - 1)p_{33}(t), \\
c_4 &= u_4(\theta_1, \theta_2, \theta_3, t) = K(\theta_1, \theta_2, \theta_3, t) - (e^{\theta_1} - 1)\delta_1(t) \\
&\quad - (e^{\theta_2} - 1)\delta_2(t) - (e^{\theta_3} - 1)\delta_3(t), \tag{6}
\end{aligned}$$

where

$$p_{11}(t) = \exp \left\{ - \int_0^t \lambda_{01}(z) dz \right\},$$

$$p_{22}(t) = \exp \left\{ - \int_0^t [\lambda_{12}(z) + \lambda_{02}(z)] dz \right\},$$

$$p_{33}(t) = \exp \left\{ - \int_0^t [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz \right\},$$

$$p_{12}(t) = \int_0^t \lambda_{12}(t_1) \exp \left\{ - \int_0^{t_1} [\lambda_{12}(z) + \lambda_{02}(z)] dz - \int_{t_1}^t \lambda_{01}(z) dz \right\} dt_1,$$

$$p_{13}(t) = \int_0^t \int_{t_2}^t \lambda_{12}(t_1) \lambda_{23}(t_2) \exp \left\{ - \int_0^{t_2} [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz \right. \\$$

$$\left. - \int_{t_2}^{t_1} [\lambda_{12}(z) + \lambda_{02}(z)] dz - \int_{t_1}^t \lambda_{01}(z) dz \right\} dt_1 dt_2$$

$$+ \int_0^t \lambda_{13}(t_2) \exp \left\{ - \int_0^{t_2} [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz \right.$$

$$\left. - \int_{t_2}^t \lambda_{01}(z) dz \right\} dt_2,$$

$$p_{23}(t) = \int_0^t \lambda_{23}(t_2) \exp \left\{ - \int_0^{t_2} [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz \right. \\$$

$$\left. - \int_{t_2}^t [\lambda_{12}(z) + \lambda_{02}(z)] dz \right\} dt_2,$$

$$\delta_1(t) = \int_0^t \lambda_{10}(t_3) \exp \left\{ - \int_{t_3}^t [\lambda_{01}(z) dz] \right\} dt_3 + \int_0^t \int_{t_3}^t \lambda_{20}(t_3) \lambda_{12}(t_1)$$

$$\exp \left\{ - \int_{t_3}^{t_1} [\lambda_{12}(z) + \lambda_{02}(z)] dz - \int_{t_1}^t \lambda_{01}(z) dz \right\} dt_1 dt_3$$

$$+ \int_0^t \int_{t_3}^t \lambda_{30}(t_3) \lambda_{13}(t_2) \exp \left\{ - \int_{t_3}^{t_2} [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz \right. \\$$

$$\left. - \int_{t_2}^t \lambda_{01}(z) dz \right\} dt_2 dt_3 + \int_0^t \int_{t_3}^t \int_{t_2}^t \lambda_{30}(t_3) \lambda_{12}(t_1) \lambda_{23}(t_2)$$

$$\exp \left\{ - \int_{t_3}^{t_2} [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz - \int_{t_2}^{t_1} [\lambda_{12}(z) + \lambda_{02}(z)] dz \right. \\ \left. - \int_{t_1}^t \lambda_{01}(z) dz \right\} dt_1 dt_2 dt_3,$$

$$\delta_2(t) = \int_0^t \lambda_{20}(t_3) \exp \left\{ - \int_{t_3}^t [\lambda_{12}(z) + \lambda_{02}(z)] dz \right\} dt_3$$

$$+ \int_0^t \int_{t_3}^t \lambda_{30}(t_3) \lambda_{23}(t_2) \exp \left\{ - \int_{t_3}^{t_2} [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz \right. \\ \left. - \int_{t_2}^t [\lambda_{12}(z) + \lambda_{02}(z)] dz \right\} dt_2 dt_3$$

and

$$\delta_3(t) = \int_0^t \lambda_{30}(t_3) \exp \left\{ - \int_{t_3}^t [\lambda_{13}(z) + \lambda_{23}(z) + \lambda_{03}(z)] dz \right\} dt_3.$$

These four arbitrary constants (6) are the independent integrals which, according to characteristic theory, can be related by the functional relationship

$$u_4(\theta_1, \theta_2, \theta_3, t) = \psi(u_1(\theta_1, \theta_2, \theta_3, t), u_2(\theta_1, \theta_2, \theta_3, t), \\ u_3(\theta_1, \theta_2, \theta_3, t)). \quad (7)$$

The exact functional form of ψ can be identified if the initial conditions of the model are known. For this purpose, assume $X_1(0)$,

$x_2(0)$ and $x_3(0)$ have the joint cumulant generating function $k(\theta_1, \theta_2, \theta_3)$,

$$\text{i.e. } K(\theta_1, \theta_2, \theta_3, 0) = k(\theta_1, \theta_2, \theta_3).$$

Also when $t = 0$ the system of equations (6) becomes

$$u_1(\theta_1, \theta_2, \theta_3, 0) = e^{\theta_1 - 1},$$

$$u_2(\theta_1, \theta_2, \theta_3, 0) = e^{\theta_2 - 1},$$

$$u_3(\theta_1, \theta_2, \theta_3, 0) = e^{\theta_3 - 1},$$

$$u_4(\theta_1, \theta_2, \theta_3, 0) = k(\theta_1, \theta_2, \theta_3). \quad (8)$$

So when $t = 0$, equation (7) reduces to

$$k(\theta_1, \theta_2, \theta_3) = \psi(e^{\theta_1 - 1}, e^{\theta_2 - 1}, e^{\theta_3 - 1}). \quad (9)$$

Now letting $y_i = e^{\theta_i - 1}$ for $i = 1, 2, 3$, (9) can be rewritten

$$k(\ln(y_1 + 1), \ln(y_2 + 1), \ln(y_3 + 1)) = \psi(y_1, y_2, y_3). \quad (10)$$

Equation (10) gives the functional form of ψ in terms of the initial joint cumulant generating function. Using this form for ψ , equation (7) becomes

$$u_4(\theta_1, \theta_2, \theta_3, t) = k \ln(u_1(\theta_1, \theta_2, \theta_3, t) + 1), \ln(u_2(\theta_1, \theta_2, \theta_3, t) + 1), \\ \ln(u_3(\theta_1, \theta_2, \theta_3, t) + 1)). \quad (11)$$

The solution to (2) is now obtained by substituting (6) into (11) and solving for $K(\theta_1, \theta_2, \theta_3, t)$. This results in

$$K(\theta_1, \theta_2, \theta_3, t) = k \left[\ln(1 + (e^{\theta_1 - 1}) p_{11}(t)), \ln(1 + \sum_{i=1}^2 (e^{\theta_i - 1}) p_{i2}(t)), \right. \\ \left. \ln(1 + \sum_{i=1}^3 (e^{\theta_i - 1}) p_{i3}(t)) \right] \\ + \sum_{i=1}^3 (e^{\theta_i - 1}) \delta_i(t) \quad (12)$$

where the $p_{ij}(t)$ and $\delta_i(t)$ are defined in (6).

2.1.3 The Moments of the Mixed Three-Compartment Distribution

The moments of the distribution can now be found by differentiating the cumulant generating function (12) with respect to the appropriate parameters and evaluating the partial derivatives at $\theta_i = 0$ for all i . Defining μ_i and σ_{ii} to be the mean and variance of $X_i(0)$ for $i = 1, 2$ and 3 and σ_{ij} to be the covariance of $X_i(0)$ and $X_j(0)$, $i, j = 1, 2, 3$, $i \neq j$, then the moments are given by

$$\begin{aligned}
 E(X_i(t)) &= \sum_{k=1}^3 \mu_k p_{ik}(t) + \delta_i(t), \\
 V(X_i(t)) &= \sum_{k=1}^3 \sum_{\ell=1}^3 [\sigma_{k\ell} p_{i\ell}(t) p_{ik}(t)] \\
 &\quad + \mu_k p_{ik}(t)(1-p_{ik}(t)) + \delta_i(t), \\
 \text{cov}[X_i(t), X_j(t)] &= \sum_{k=1}^3 \sum_{\ell=j}^3 \sigma_{k\ell} p_{j\ell}(t) p_{ik}(t) \\
 &\quad - \sum_{\ell=\max[i,j]}^3 \mu_\ell p_{i\ell}(t) p_{j\ell}(t). \tag{13}
 \end{aligned}$$

These results are a generalization of the 2-compartment catenary model and the 3-compartment mammillary model of Cardenas and Matis [1974]. See Appendix B for the details of this derivation.

2.2 The n-Compartment Mixed Catenary-Mammillary Model

2.2.1 The Partial Differential Equation for the Cumulant Generating Function

The 3-compartment mixed model will now be extended to n compartments. The derivations of the joint cumulant generating function and the moments of the distribution are completely analogous to those of the 3-compartment case. Figure 7, page 17, illustrates the n-compartment mixed model under consideration.

The transition probabilities are:

Prob {a single unit enters compartment i from outside the system in the interval

$$(t, t+\Delta t)} = \lambda_{10}(t)\Delta t + o(\Delta t) \text{ for } i=1, 2, \dots, n,$$

Prob {a single unit moves from compartment j to compartment i in the interval (t, t+\Delta t)} =

$$x_j(t)\lambda_{ij}(t)\Delta t + o(\Delta t) \text{ for } j=1, 2, \dots, n$$

and $i=0, 1, 2, \dots, n$.

There are $4n-3$ events with probability of first order magnitude of Δt and the probability of these events will be

$$\text{Prob } \{\Delta X_1(t)=k_1, \Delta X_2(t)=k_2, \dots, \Delta X_n(t)=k_n | X_1(t), \dots, X_n(t)\} =$$

$$\left\{ \begin{array}{l} x_n(t)\lambda_{in}(t)\Delta t + o(\Delta t) \quad k_i=+1, \quad k_n=-1 \quad i=1, 2, \dots, n-1 \\ \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \text{all other } k's \text{ are zero.} \\ x_i(t)\lambda_{0i}(t)\Delta t + o(\Delta t) \quad k_i=-1 \quad i=1, 2, \dots, n \\ \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \text{all other } k's \text{ are zero.} \\ x_i(t)\lambda_{i-1,i}(t)\Delta t + o(\Delta t) \quad k_{i-1}=+1, \quad k_i=-1 \quad i=2, 3, \dots, n-1 \\ \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \text{all other } k's \text{ are zero.} \\ \lambda_{10}(t)\Delta t + o(\Delta t) \quad k_i=+1 \quad i=1, 2, \dots, n \\ \qquad \qquad \qquad \qquad \qquad \qquad \qquad \qquad \text{all other } k's \text{ are zero.} \end{array} \right.$$

The differential equation for the joint cumulant generating function can now be written

$$\begin{aligned}
 \frac{\partial K(\theta, t)}{\partial t} &= (e^{-\theta_1} - 1) \lambda_{01}(t) \frac{\partial K(\theta, t)}{\partial \theta_1} \\
 &+ \sum_{i=2}^{n-1} \left[(e^{-\theta_i + \theta_{i-1}} - 1) \lambda_{i-1, i}(t) + (e^{-\theta_i} - 1) \lambda_{0i}(t) \frac{\partial K(\theta, t)}{\partial \theta_i} \right] \\
 &+ \left[(e^{-\theta_n} - 1) \lambda_{0n}(t) + \sum_{i=1}^{n-1} (e^{-\theta_i - \theta_n} - 1) \lambda_{in}(t) \right] \frac{\partial K(\theta, t)}{\partial \theta_n} \\
 &+ \sum_{i=1}^n (e^{-\theta_i} - 1) \lambda_{i0}(t),
 \end{aligned} \tag{14}$$

where $K(\theta, t)$ denotes $K(\theta_1, \theta_2, \dots, \theta_n, t)$.

2.2.2 The Joint Cumulant Generating Function

The subsidiary equations associated with equation (14) are

$$\begin{aligned}
 \frac{dt}{1} &= \frac{d\theta_1}{(1-e^{-\theta_1})\lambda_{01}(t)} = \frac{d\theta_1}{(1-e^{-\theta_{i-1}-\theta_i})\lambda_{i-1, i}(t)+(1-e^{-\theta_i})\lambda_{0i}(t)} \\
 &= \frac{d\theta_n}{(1-e^{-\theta_n})\lambda_{0n}(t)+\sum_{i=1}^{n-1} (1-e^{-\theta_i-\theta_n})\lambda_{in}(t)} \\
 &= \frac{dK(\theta, t)}{\sum_{i=1}^n (e^{-\theta_i} - 1) \lambda_{i0}(t)} \quad \text{for } i=2, 3, \dots, n-1.
 \end{aligned} \tag{15}$$

Letting $V_i = e^{\theta_i} - 1$ for $i = 1, 2, \dots, n$ the subsidiary equations can be rewritten

$$\begin{aligned}
 dv_1 &= v_1 \lambda_{01}(t) dt, \\
 dv_i &= [(v_{i-1} - v_i) \lambda_{i-1,i}(t) + F_i \lambda_{0i}(t)] dt, \quad i=2,3,\dots,n-1, \\
 dv_n &= \left[v_n \lambda_{0n}(t) + \sum_{i=1}^{n-1} (v_n - v_i) \lambda_{in}(t) \right] dt, \\
 dK(\theta, t) &= \sum_{i=1}^n v_i \lambda_{i0}(t) dt. \tag{16}
 \end{aligned}$$

This system can now be solved sequentially for v_i , $i=1,2,\dots,n$ and $K(\theta, t)$ in terms of the transition rates $\lambda_{ij}(t)$ and $n+1$ constants of integration. Solving this system for the constants of integration and replacing v_i by $(e^{\theta_i} - 1)$ one obtains

$$\begin{aligned}
 c_1 &= u_1(\theta, t) = (e^{\theta_1} - 1) \exp\{-g_1(t, 0)\}, \\
 c_2 &= u_2(\theta, t) = (e^{\theta_2} - 1) \exp\{-g_2(t, 0)\} \\
 &\quad + (e^{\theta_1} - 1) \int_0^t \lambda_{12}(t_1) \exp\{-g_1(t, t_1) - g_2(t_1, 0)\} dt_1, \\
 &\vdots \\
 c_i &= u_i(\theta, t) = (e^{\theta_i} - 1) \exp\{-g_i(t, 0)\} \\
 &\quad + (e^{\theta_{i-1}} - 1) \int_0^t \lambda_{i-1,i}(t_{i-1}) \exp\{-g_{i-1}(t, t_{i-1}) \\
 &\quad \quad \quad - g_i(t_{i-1}, 0)\} dt_{i-1} \\
 &\quad + \sum_{k=1}^{i-2} (e^{\theta_k} - 1) \int_0^t \int_{t_{i-1}}^{t_k} \dots \int_{t_{k+1}}^{t_k} r_{ki}(t_k, \dots, t_{i-1})
 \end{aligned}$$

$$\exp\{-g_\ell(t, t_\ell) - \sum_{k=\ell+1}^{i-1} g_k(t_{k-1}, t_k) - g_i(t_{i-1}, 0)\} \prod_{k=\ell}^{i-1} dt_k$$

for $i = 3, 4, \dots, n-1$,

$$C_n = u_n(\underline{\theta}, t) = (e^{\theta_{n-1}}) \exp\{-g_n(t, 0)\}$$

$$+ (e^{\theta_{n-1}}) \int_0^t \lambda_{n-1, n}(t_{n-1}) \exp\{-g_{n-1}(t, t_{n-1})$$

$$-g_n(t_{n-1}, 0)\} dt_{n-1}$$

$$+ \sum_{\ell=1}^{n-2} (e^{\theta_\ell}) \left[\int_0^t \lambda_{\ell, n}(t_{n-1}) \exp\{-g_\ell(t, t_{n-1}) - g_n(t_{n-1}, 0)\} dt_{n-1} \right]$$

$$+ \sum_{m=1}^{n-\ell-1} \int_0^t \int_{t_{n-1}}^t \dots \int_{t_{\ell+1}}^t \lambda_{\ell+m, n}(t_{n-1}) \Gamma_{\ell, \ell+m}(t_\ell, \dots, t_{\ell+m-1})$$

$$\exp\{-g_\ell(t, t_\ell) - \sum_{k=\ell+1}^{l+m} g_k(t_{k-1}, t_k) - g_n(t_{n-1}, 0)\} \prod_{k=\ell}^{l+m-1} dt_k dt_{n-1} \Big],$$

$$C_{n+1} = u_{n+1}(\underline{\theta}, t) = K(\underline{\theta}, t) - \sum_{j=1}^n (e^{\theta_j}) \left[\int_0^t \lambda_{j0}(t_n) \exp\{-g_j(t, t_n)\} dt_n \right]$$

$$+ \int_0^t \int_{t_n}^t \lambda_{j+1, 0}(t_n) \lambda_{j, j+1}(t_j) \exp\{-g_j(t, t_j) - g_{j+1}(t_j, t_n)\} dt_j dt_n$$

$$+ \sum_{\ell=2}^{n-j-1} \int_0^t \int_{t_n}^t \dots \int_{t_{j+1}}^t \lambda_{j+\ell, 0}(t_n) \Gamma_{j, j+\ell}(t_j, \dots, t_{j+\ell-1}) \exp\{-g_j(t, t_j)\}$$

$$- \sum_{k=j+1}^{j+\ell-1} g_k(t_{k-1}, t_k) - g_{j+\ell}(t_{j+\ell-1}, t_n) \} \prod_{k=j}^{j+\ell-1} dt_k dt_n$$

$$+ \int_0^t \int_{t_n}^t \lambda_{n0}(t_n) \lambda_{jn}(t_{n-1}) \exp\{-g_j(t, t_{n-1}) - g_n(t_{n-1}, t_n)\} dt_{n-1} dt_n$$

$$\begin{aligned}
 & + \sum_{\ell=1}^{n-j-1} \int_0^t \int_{t_n}^t \dots \int_{t_{j+1}}^t \lambda_{n0}(t_n) \Gamma_{j,j+\ell}(t_j, \dots, t_{j+\ell-1}) \lambda_{j+\ell,n}(t_{n-1}) \\
 & \exp\{-g_j(t, t_j) - \sum_{k=j+1}^{j+\ell} g_k(t_{k-1}, t_k) - g_n(t_{n-1}, t_n)\} \prod_{k=j}^{j+\ell-1} dt_k dt_{n-1} dt_n,
 \end{aligned} \tag{17}$$

where $g_1(x, y) = \int_y^x \lambda_{01}(z) dz,$

$$g_i(x, y) = \int_y^x [\lambda_{0i}(z) + \lambda_{i-1,i}(z)] dz, \quad i=2, 3, \dots, n-1,$$

$$g_n(x, y) = \int_y^x \sum_{j=0}^{n-1} \lambda_{jn}(z) dz$$

and $\Gamma_{ij}(z_1, \dots, z_{j-i}) = \lambda_{i,i+1}(z_1) \dots \lambda_{j-1,j}(z_{j-1}).$

These $n+1$ constants can now be related by some function ϕ such that

$$u_{n+1}(\underline{\theta}, t) = \phi(u_1(\underline{\theta}, t), \dots, u_n(\underline{\theta}, t)) \tag{18}$$

where ϕ is determined by the initial conditions. Assume the initial distribution $x_1(0), x_2(0), \dots, x_n(0)$ has the joint cumulant generating function

$$K(\theta_1, \theta_2, \dots, \theta_n, 0) = k(\theta_1, \theta_2, \dots, \theta_n). \tag{19}$$

Now one can verify that the joint cumulant generating function of the stochastic vector $X_1(t), \dots, X_n(t)$ at any time t is given by

$$K(\theta_1, \theta_2, \dots, \theta_n, t) = k \left\{ \ln[1 + (e^{\theta_1} - 1)p_{11}(t)], \ln[1 + \sum_{i=1}^2 (e^{\theta_i} - 1)p_{12}(t)], \dots, \ln[1 + \sum_{i=1}^j (e^{\theta_i} - 1)p_{1j}(t)], \dots, \right. \\ \left. \ln[1 + \sum_{i=1}^n (e^{\theta_i} - 1)p_{1n}(t)] \right\} + \sum_{j=1}^n (e^{\theta_j} - 1)\delta_j(t), \quad (20)$$

where

$$p_{ii}(t) = \exp\{-g_i(t, 0)\}, \quad i = 1, \dots, n,$$

$$p_{\ell i}(t) = \int_0^t \int_{t_{\ell-1}}^t \dots \int_{t_{\ell+1}}^t r_{\ell i}(t_\ell, \dots, t_{i-1}) \exp\{-g_\ell(t, t_\ell) - \sum_{k=\ell+1}^{i-1} g_k(t_{k-1}, t_k) - g_i(t_{i-1}, 0)\} \prod_{k=\ell}^{i-1} dt_k,$$

for $i = 2, 3, \dots, n-1; \ell = 1, 2, \dots, i-1$.

$$p_{\ell n}(t) = \int_0^t \lambda_{\ell n}(t_{n-1}) \exp\{-g_\ell(t, t_{n-1}) - g_n(t_{n-1}, 0)\} dt_{n-1} \\ + \sum_{m=1}^{n-\ell-1} \int_0^t \int_{t_{n-1}}^t \dots \int_{t_{\ell+1}}^t \lambda_{\ell+m, n}(t_{n-1}) r_{\ell, \ell+m}(t_\ell, \dots, t_{\ell+m-1}) \\ \exp\{-g_\ell(t, t_\ell) - \sum_{k=\ell+1}^{\ell+m} g_k(t_{k-1}, t_k) - g_n(t_{n-1}, 0)\} \prod_{k=\ell}^{\ell+m-1} dt_k dt_{n-1},$$

for $\ell = 1, 2, \dots, n-1$,

and

$$\begin{aligned}
 \delta_j(t) = & \int_0^t \lambda_{j0}(t_n) \exp\{-g_j(t, t_n)\} dt_n + \int_0^t \int_{t_n}^t \lambda_{j+1,0}(t_n) \lambda_{j,j+1}(t_j) \\
 & \exp\{-g_j(t, t_j) - g_{j+1}(t_j, t_n)\} dt_j dt_n \\
 & + \sum_{\ell=2}^{n-j-1} \int_0^t \int_{t_n}^t \cdots \int_{t_{j+1}}^t \lambda_{j+\ell,0}(t_n) \Gamma_{j,j+\ell}(t_j, \dots, t_{j+\ell-1}) \\
 & \exp\{-g_j(t, t_j) - \sum_{k=j+1}^{j+\ell-1} g_k(t_{k-1}, t_k) - g_{j+\ell}(t_{j+\ell-1}, t_n)\} \prod_{k=j}^{j+\ell-1} dt_k dt_n \\
 & + \int_0^t \int_{t_n}^t \lambda_{n0}(t_n) \lambda_{jn}(t_{n-1}) \exp\{-g_j(t, t_{n-1}) - g_n(t_{n-1}, t_n)\} dt_{n-1} dt_n \\
 & + \sum_{\ell=1}^{n-j-1} \int_0^t \int_{t_n}^t \cdots \int_{t_{j+1}}^t \lambda_{n0}(t_n) \Gamma_{j,j+\ell}(t_j, \dots, t_{j+\ell-1}) \lambda_{j+\ell,n}(t_{n-1}) \\
 & \exp\{-g_j(t, t_j) - \sum_{k=j+1}^{j+\ell} g_k(t_{k-1}, t_k) - g_n(t_{n-1}, t_n)\} \prod_{k=j}^{j+\ell-1} dt_k dt_{n-1} dt_n
 \end{aligned}$$

where $g_i(x, y)$ and $\Gamma_{ij}(z_1, \dots, z_{j-i})$ are defined in (17).

2.2.3 The Moments of the Mixed n-Compartment Distribution

The moments derived from this cumulant generating function (20) are the logical extension of those derived for the 3-compartment model. As before, define μ_i and σ_{ii} to be the mean and variance of $X_i(0)$ for all i , and σ_{ij} to be the covariance of $X_i(0)$ and $X_j(0)$ for all i and j , $i \neq j$. (See Appendix B for the details.) One obtains

$$E(X_i(t)) = \sum_{k=1}^n \mu_k p_{ik}(t) + \delta_i(t), \quad i=1, 2, \dots, n,$$

$$V(X_i(t)) = \sum_{k=1}^n \left\{ \sum_{l=1}^n \sigma_{lk} p_{il}(t) p_{ik}(t) + \mu_k p_{ik}(t)(1-p_{ik}(t)) \right\} + \delta_i(t), \\ i=1, 2, \dots, n,$$

$$\text{cov}(X_i(t), X_j(t)) = \sum_{k=1}^n \sum_{l=j}^n \sigma_{kl} p_{jl}(t) p_{ik}(t) - \sum_{l=\max[i,j]}^n \mu_l p_{il}(t) p_{jl}(t), \\ i, j=1, 2, \dots, n \quad i \neq j, \quad (21)$$

where $p_{ij}(t)$ and $\delta_i(t)$ are defined in (20) for all i and j .

Higher order moments may be obtained by a straightforward extension of this procedure to higher derivatives.

2.3 A Special Case

It is frequently true that the initial number of units in each compartment is known. For example, in the gastrointestinal model cited in Section 1.2, it was known that the rumen contained 4,000 beads at time zero while the two other compartments contained no beads.

If the initial distribution is known to be $X_i(0) = x_i$ for $i=1, 2, \dots, n$ then $K(\underline{\theta}, 0) = k(\underline{\theta}) = x_1 \theta_1 + x_2 \theta_2 + \dots + x_n \theta_n$. Now the cumulant generating function can be written from equation (20). This becomes

$$K(\underline{\theta}, t) = \sum_{j=1}^n x_j \ln [1 + \sum_{i=1}^j (e^{\theta_i} - 1) p_{ij}(t)] \\ + \sum_{j=1}^n (e^{\theta_j} - 1) \delta_j(t)$$

where the $p_{ij}(t)$ and $\delta_j(t)$ are defined in (20).

Matis [1970] discusses a cumulant generating function of this form extensively and shows it is associated with a sum of n independent multinomial distributions and a sum of n independent Poisson distributions. Establishing this, one can then appeal to the unique form of the generating function and realize a physical interpretation of the $p_{ij}(t)$ and $\delta_j(t)$ parameters. This is

$p_{ij}(t) = \text{Prob} \{ \text{a unit which was in compartment } j \text{ at time } t=0, \text{ is in compartment } i \text{ at time } t \},$

$\delta_j(t) = \text{The expected number of units in compartment } j \text{ at time } t \text{ which were not in the system at time } t = 0.$

This result is very important in the later development of applications using compartmental analysis.

3. THE GENERAL IRREVERSIBLE TIME-DEPENDENT MODEL

The n-compartment mixed catenary-mammillary model derived in the previous section is further generalized in this section. The assumption is made that a unit in the first compartment can transfer to any one of the remaining n-1 compartments and a unit in the second compartment can transfer to any one of the remaining n-2 compartments and so on. In addition, a unit can enter or leave the system through any compartment. This arrangement is illustrated in Figure 9. Under the assumptions in Section 1.4, such a structure is the most general possible irreversible time-dependent model.

3.1 The n-Compartment General Model

3.1.1 The Partial Differential Equation for the Cumulant Generating Function

The possible transition probabilities can be summarized:

Prob {single unit moves from compartment j to compartment i in the interval $(t, t+\Delta t)$ } = $x_j(t)\lambda_{ij}(t)\Delta t + o(\Delta t)$
for $j=2, 3, \dots, n$ and $i=1, 2, \dots, j-1$.

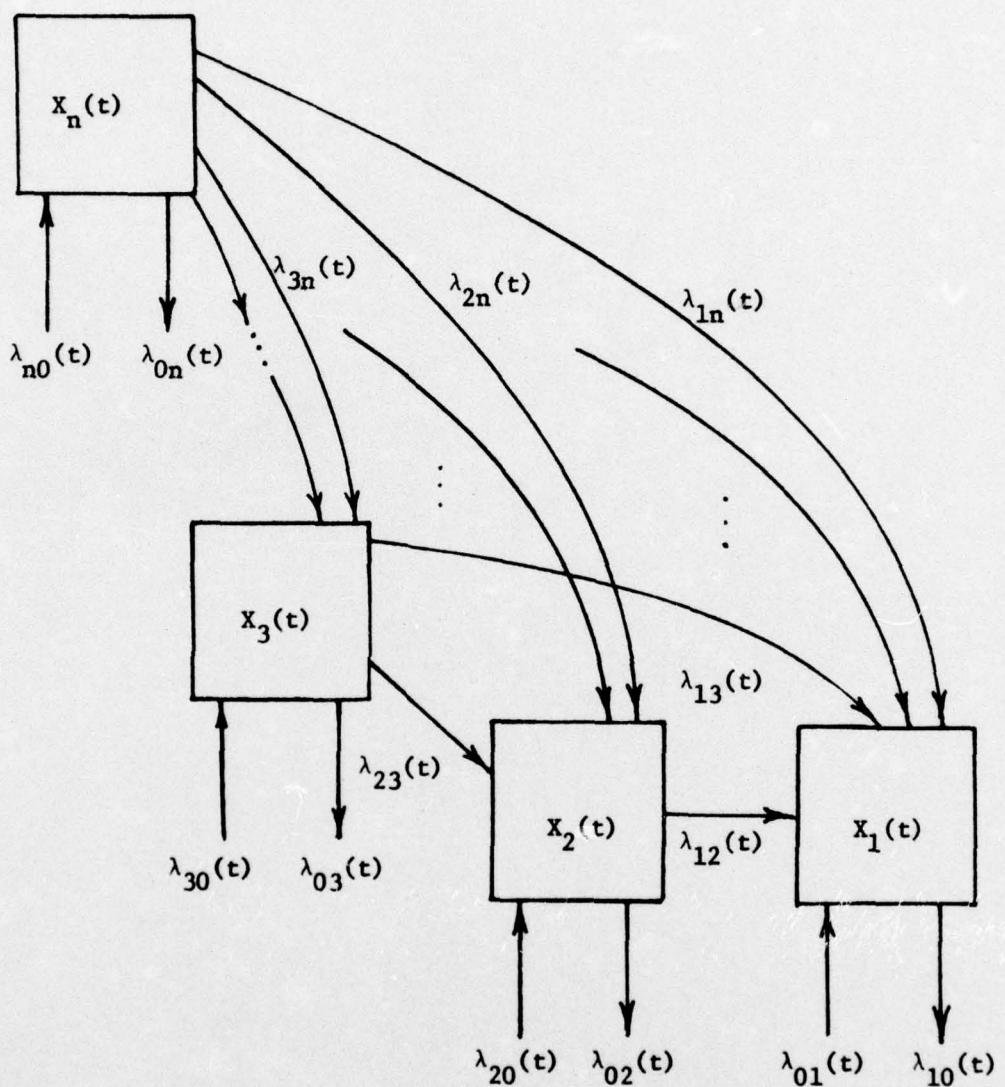


Figure 9

General n -Compartment Irreversible Model

Prob {single unit in compartment j leaves the system
in the interval $(t, t+\Delta t)$ } =

$$x_j(t)\lambda_{0j}(t)\Delta t + o(\Delta t) \text{ for all } j.$$

Prob {single unit enters compartment j from outside
the system in the interval $(t, t+\Delta t)$ } =

$$\lambda_{j0}(t)\Delta t + o(\Delta t) \text{ for all } j.$$

In this model there are $(n^2+3n)/2$ events with probability of first order magnitude. These events lead to the following probability statement.

Prob $\{\Delta X_1(t)=k_1, \Delta X_2(t)=k_2, \dots, \Delta X_n(t)=k_n | X_1(t), X_2(t), \dots, X_n(t)\} =$

$$\begin{cases} x_j(t)\lambda_{0j}(t)\Delta t + o(\Delta t) & k_j = -1 \text{ for } j=1, 2, \dots, n \\ & \text{and all other } k \text{'s are zero.} \\ x_j(t)\lambda_{ij}(t)\Delta t + o(\Delta t) & k_j = -1, k_i = +1 \text{ for } j=2, 3, \dots, n \text{ and} \\ & i=1, 2, \dots, j-1. \\ \lambda_{j0}(t)\Delta t + o(\Delta t) & k_j = +1 \text{ for } j=1, 2, \dots, n \\ & \text{and all other } k \text{'s are zero.} \end{cases}$$

Now proceeding as in the mixed model the multivariate distribution of the n-vector $(X_1(t), X_2(t), \dots, X_n(t))$ will be determined by finding its cumulant generating function $K(\theta_1, \theta_2, \dots, \theta_n, t)$. Denote this by $K(\underline{\theta}, t)$. The partial differential equation for $K(\underline{\theta}, t)$ can be shown to be

$$\begin{aligned} \frac{\partial K(\theta, t)}{\partial t} &= (e^{-\theta} - 1) \lambda_{01}(t) \frac{\partial K(\theta, t)}{\partial \theta_1} + \sum_{j=2}^n \sum_{i=1}^{j-1} (e^{-\theta_j} - 1) \lambda_{ij}(t) \\ &\quad + (e^{-\theta_j} - 1) \lambda_{0j}(t) \frac{\partial K(\theta, t)}{\partial \theta_j} + \sum_{j=1}^n (e^{-\theta_j} - 1) \lambda_{j0}(t). \end{aligned} \quad (22)$$

3.1.2 The Joint Cumulant Generating Function

The details of the solution to (22) are found in Appendix A. The method is the same as that used in solving (2). The solution is

$$\begin{aligned} K(\theta, t) &= k \left[\ln[1 + (e^{-\theta} - 1)p_{11}(t)], \ln[1 + \sum_{i=1}^2 (e^{-\theta_i} - 1)p_{i2}(t)], \dots, \right. \\ &\quad \left. \ln[1 + \sum_{i=1}^j (e^{-\theta_i} - 1)p_{ij}(t)], \dots, \ln[1 + \sum_{i=1}^n (e^{-\theta_i} - 1)p_{in}(t)] \right] \\ &\quad + \sum_{j=1}^n (e^{-\theta_j} - 1) \delta_j(t) \end{aligned} \quad (23)$$

where $K(\theta_1, \theta_2, \dots, \theta_n, 0) = k(\theta_1, \theta_2, \dots, \theta_n)$,

$$p_{11}(t) = \exp\{-h_1(t, 0)\}, \quad i=1, 2, \dots, n,$$

$$p_{i,i+1}(t) = \int_0^t \lambda_{i,i+1}(t_i) \exp\{-h_i(t, t_i) - h_{i+1}(t_i, 0)\} dt_i, \quad i=1, 2, \dots, n-1,$$

$$p_{1j}(t) = \int_0^t \lambda_{1j}(t_{j-1}) \exp\{-h_1(t, t_{j-1}) - h_j(t_{j-1}, 0)\} dt_{j-1}$$

$$+ \sum_{l=i+1}^{j-1} \int_0^t \int_{t_{j-1}}^t \lambda_{1l}(t_{l-1}) \lambda_{lj}(t_{j-1}) \exp\{-h_1(t, t_{l-1})\}$$

$$-h_{\lambda}(t_{\lambda-1}, t_{j-1}) - h_j(t_{j-1}, 0) \} dt_{\lambda-1} dt_{j-1} + \dots$$

$$+ \sum_{i < \lambda_1 < \lambda_2 < \dots < \lambda_{m-1} < j} \int_0^t \int_{t_{j-1}}^t \dots \int_{t_{\lambda_2-1}}^t \lambda_{i \lambda_1}(\lambda_{\lambda_1-1})$$

$$\prod_{i=1}^{m-2} (\lambda_{\lambda_1, \lambda_{i+1}}(t_{\lambda_{i+1}-1})) \lambda_{\lambda_{m-1}, j}(t_{j-1}) \exp\{-h_i(t, t_{\lambda_1-1})\}$$

$$- \sum_{i=1}^{m-2} h_{\lambda_1}(t_{\lambda_1-1}, t_{\lambda_{i+1}-1}) - h_j(t_{j-1}, 0) \} \prod_{i=1}^{m-1} dt_{\lambda_1-1} dt_{j-1} + \dots$$

$$+ \int_0^t \int_{t_{j-1}}^t \dots \int_{t_{i+1}}^t r_{ij}(t_i, t_{i+1}, \dots, t_{j-1}) \exp\{-h_i(t, t_i)\}$$

$$- \sum_{\lambda=i+1}^{j-1} h_{\lambda}(t_{\lambda-1}, t_{\lambda}) - h_j(t_{j-1}, 0) \} \prod_{\lambda=1}^{j-1} dt_{\lambda},$$

$j=3, 4, \dots, n$ and $i=1, \dots, j-2$,

$$\delta_n(t) = \int_0^t \lambda_{n0}(t_n) \exp\{-h_n(t, t_n)\} dt_n,$$

$$\delta_{n-1}(t) = \int_0^t \lambda_{n-1,0}(t_n) \exp\{-h_{n-1}(t, t_n)\} dt_n + \int_0^t \int_{t_n}^t \lambda_{n0}(t_n) \lambda_{n-1,n}(t_{n-1})$$

$$\exp\{-h_{n-1}(t, t_{n-1}) - h_n(t_{n-1}, t_n)\} dt_{n-1} dt_n,$$

$$\delta_{n-2}(t) = \int_0^t \lambda_{n-2,0}(t_n) \exp\{-h_{n-2}(t, t_n)\} dt_n$$

$$+ \int_0^t \int_{t_n}^t \lambda_{n-1,0}(t_n) \lambda_{n-2,n-1}(t_{n-2}) \exp\{-h_{n-2}(t, t_{n-2})$$

$$- h_{n-1}(t_{n-2}, t_n)\} dt_{n-2} dt_n + \int_0^t \int_{t_n}^t \lambda_{n0}(t_n) \lambda_{n-2,n}(t_{n-1})$$

$$\exp\{-h_{n-2}(t, t_{n-1}) - h_n(t_{n-1}, t_n)\} dt_{n-1} dt_n$$

$$\begin{aligned}
& + \int_0^t \int_{t_n}^t \int_{t_{n-1}}^t \lambda_{n0}(t_n) \lambda_{n-2,n-1}(t_{n-2}) \lambda_{n-1,n}(t_{n-1}) \\
& \exp\{-h_{n-2}(t, t_{n-2}) - h_{n-1}(t_{n-2}, t_{n-1}) - h_n(t_{n-1}, t_n)\} dt_{n-2} dt_{n-1} dt_n.
\end{aligned}$$

In general

$$\begin{aligned}
\delta_j(t) = & \int_0^t \lambda_{j0}(t_n) \exp\{-h_j(t, t_n)\} dt_n + \sum_{i=j+1}^n \int_0^t \int_{t_n}^t \lambda_{i0}(t_n) \lambda_{ji}(t_{i-1}) \\
& \exp\{-h_j(t, t_{i-1}) - h_i(t_{i-1}, t_n)\} dt_{i-1} dt_n \\
& + \sum_{\ell=2}^{n-j} \sum_{k=j+1}^{j+\ell-1} \int_0^t \int_{t_n}^t \int_{t_{j+\ell-1}}^t \lambda_{j+\ell,0}(t_n) \lambda_{j,k}(t_{k-1}) \lambda_{k,j+\ell}(t_{j+\ell-1}) \\
& \exp\{-h_j(t, t_{k-1}) - h_k(t_{k-1}, t_{j+\ell-1}) - h_{j+\ell}(t_{j+\ell-1}, t_n)\} \\
& dt_{k-1} dt_{j+\ell-1} dt_n + \dots \\
& + \sum_{j<\ell_1<\ell_2<\dots<\ell_{m-1}} \int_0^t \int_{t_n}^t \int_{t_{\ell_{m-1}-1}}^t \dots \int_{t_{\ell_2-1}}^t \lambda_{\ell_{m-1},0}(t_n) \lambda_{j,\ell_1}(t_{\ell_1-1}) \\
& \prod_{i=1}^{m-2} \lambda_{\ell_i,\ell_{i+1}}(t_{\ell_{i+1}-1}) \exp\{-h_j(t, t_{\ell_1-1}) - \sum_{i=1}^{m-2} h_{\ell_i}(t_{\ell_i-1}, t_{\ell_{i+1}-1}) \\
& - h_{\ell_{m-1}}(t_{\ell_{m-1}-1}, t_n)\} \prod_{i=1}^{m-1} dt_{\ell_i-1} dt_n + \dots \\
& + \int_0^t \int_{t_n}^t \dots \int_{t_{j+2}}^t \int_{t_{j+1}}^t \lambda_{n0}(t_n) \Gamma_{jn}(t_j, t_{j+1}, \dots, t_{n-1}) \\
& \exp\{-h_j(t, t_j) - \sum_{i=j}^{n-1} h_{i+1}(t_i, t_{i+1})\} \prod_{i=j}^n dt_i.
\end{aligned}$$

where

$$h_i(x, y) = \int_y^x \sum_{j=0}^{i-1} \lambda_{ji}(z) dz$$

and

$$\Gamma_{ij}(z_1, \dots, z_{j-i}) = \lambda_{i,i+1}(z_1) \dots \lambda_{j-1,j}(z_{j-i}).$$

This result is a generalization of the n-compartment mixed model derived in Section 2.2.

3.1.3 The Structure of $p_{ij}(t)$ and $\delta_j(t)$

It is evident $p_{ij}(t)$ and $\delta_j(t)$ are lengthy, complex expressions and this complexity increases rapidly with an increase in the number of compartments.

But the structure of these terms can readily be seen by considering their relationship to the binomial coefficients.

As pointed out in Section 2.3, $p_{ij}(t)$ is the probability a unit in compartment j at time zero will be in compartment i at time t. Since all the possible paths from compartment j to compartment i are mutually exclusive events, $p_{ij}(t)$ must be the sum of the probability contributions from each of these. The probability of each path is expressed as a multiple integral where the multiplicity is equal to the number of transfers along that path. A given transfer is either a part of a path from compartment j to compartment i or it is not, and it is this binomial aspect which gives rise to the binomial coefficients of Figure 10. This figure is the well known arrangement of the binomial

coefficients known as Pascal's triangle. The integral structure of $p_{ij}(t)$ is given by the rows of the triangle. The diagonals counting from the left correspond to the multiplicity of the integral. For example, if $j-i=k$, then the k^{th} row indicates $p_{ij}(t)$ will have the form;

$$\begin{aligned} & (\text{one single integral}) + ((k-1) \text{ double integrals}) + \dots \\ & + \left(\binom{k-1}{m-1} m\text{-fold integrals} \right) + \dots + (\text{one } k\text{-fold integral}). \end{aligned}$$

This is a total of 2^{k-1} integrals to evaluate.

<u>$j-i$</u>			Total no. of terms
1	1	single integrals	1
2	1 1	double integrals	2
3	1 2 1	triple integrals	4
4	1 3 3 1	four-fold integrals	8
5	1 4 6 4 1	m -fold integrals	
\vdots		k -fold integrals	
k	1 $k-1$... $\binom{k-1}{m-1} \dots 1$		2^{k-1}
\vdots			
$n-1$	1 $n-2$... $\binom{n-2}{m-1} \dots 1$	($n-1$)-fold integral	2^{n-2}

Figure 10

Structure of $p_{ij}(t)$ using Pascal's Triangle

In an application of this model to reliability in Section 4 the calculation of

$$\sum_{i=1}^n p_{in}(t)$$

is required. This could contain as many as $2^{n-1}-1$ integrals to evaluate!

The structure of $\delta_j(t)$ is determined in a similar way using Pascal's triangle. For a model containing n compartments the expression for $\delta_j(t)$ contains 2^{n-j} terms. The number of integrals of a given multiplicity can be read from Figure 11. For $\delta_j(t)$ the $(n-j+1)^{th}$ row of

<u>Row</u>								
1		1						$\delta_n(t)$
2		1	1					$\delta_{n-1}(t)$
3		1	2	1				$\delta_{n-2}(t)$
4		1	3	3	1			$\delta_{n-3}(t)$
5		1	4	6	4	1		$\delta_{n-4}(t)$
:								:
$n-j+1$		1	$n-j$	\dots	$\binom{n-j}{m-1}$	\dots	1	$\delta_j(t)$
:								:
n	1	\dots	$\binom{n-1}{m-1}$	\dots		1		$\delta_1(t)$

Figure 11
Structure of $\delta_j(t)$ using Pascal's Triangle

Pascal's triangle indicates the expression will have the form;

$$\begin{aligned}
 & \left(\text{one single integral} \right) + \left((n-j) \text{ double integrals} \right) + \dots \\
 & + \left(\binom{n-j}{m-1} \text{ m-fold integrals} \right) + \dots + \left(\text{one } (n-j+1)\text{-fold integral} \right).
 \end{aligned}$$

3.1.4 The Moments of the General n-Compartment Distribution

Define μ_i and σ_{ii} to be the mean and variance of $X_i(0)$ and σ_{ij} to be the covariance of $X_i(0)$ and $X_j(0)$. Then the moments of the general n-compartment distribution can be written directly from (21). Observing that the cumulant generating functions (20) and (23) are identical in form, the moments will also be identical in form. Hence

$$\begin{aligned}
 E(X_i(t)) &= \sum_{k=1}^n \mu_k p_{ik}(t) + \delta_i(t) \quad i=1, 2, \dots, n \\
 V(X_i(t)) &= \sum_{k=1}^n \left\{ \sum_{l=1}^n \sigma_{kl} p_{il}(t) p_{ik}(t) + \mu_k p_{ik}(t) (1 - p_{ik}(t)) \right\} + \delta_i(t) \\
 &\quad i=1, 2, \dots, n \\
 \text{cov}(X_i(t), X_j(t)) &= \sum_{k=1}^n \sum_{l=j}^n \sigma_{kl} p_{jl}(t) p_{ik}(t) - \sum_{l=\max[i,j]}^n \mu_l p_{il}(t) p_{jl}(t) \\
 &\quad i, j = 1, \dots, n \quad i \neq j \quad (24)
 \end{aligned}$$

where $p_{ij}(t)$ and $\delta_i(t)$ are defined in (23) for all i and j .

Higher moments may be obtained by a simple extension of this procedure to higher derivatives. See Appendix B for the details of this derivation.

3.2 The Four-Compartment General Irreversible Model

In this section, the formulae for the general n-compartment model are shown for the special case when n=4. The cumulant generating function becomes

$$\begin{aligned}
 K(\theta_1, \theta_2, \theta_3, \theta_4, t) = k & \left[\ln[1 + (e^{\theta_1 - 1}) p_{11}(t)], \ln[1 + \sum_{i=1}^2 (e^{\theta_i - 1}) p_{i2}(t)], \right. \\
 & \ln[1 + \sum_{i=1}^3 (e^{\theta_i - 1}) p_{i3}(t)], \ln[1 + \sum_{i=1}^4 (e^{\theta_i - 1}) p_{i4}(t)] \\
 & \left. + \sum_{j=1}^4 (e^{\theta_j - 1}) \delta_j(t) \right] \quad (25)
 \end{aligned}$$

where

$$p_{11}(t) = \exp\{-h_1(t, 0)\} \quad i = 1, 2, 3, 4,$$

$$p_{12}(t) = \int_0^t \lambda_{12}(t_1) \exp\{-h_1(t, t_1) - h_2(t_1, 0)\} dt_1,$$

$$\begin{aligned}
 p_{13}(t) = & \int_0^t \lambda_{13}(t_2) \exp\{-h_1(t, t_2) - h_3(t_2, 0)\} dt_2 + \int_0^t \int_{t_2}^t \lambda_{13}(t_1, t_2) \\
 & \exp\{-h_1(t, t_1) - h_2(t_1, t_2) - h_3(t_2, 0)\} dt_1 dt_2,
 \end{aligned}$$

$$\begin{aligned}
 p_{14}(t) = & \int_0^t \lambda_{14}(t_3) \exp\{-h_1(t, t_3) - h_4(t_3, 0)\} dt_3 + \int_0^t \int_{t_3}^t \lambda_{12}(t_1) \lambda_{24}(t_3) \\
 & \exp\{-h_1(t, t_1) - h_2(t_1, t_3) - h_4(t_3, 0)\} dt_1 dt_3
 \end{aligned}$$

$$\begin{aligned}
 & + \int_0^t \int_{t_3}^t \lambda_{13}(t_2) \lambda_{34}(t_3) \exp\{-h_1(t, t_2) - h_3(t_2, t_3) - h_4(t_3, 0)\} \\
 & \quad dt_2 dt_3
 \end{aligned}$$

$$+\int_0^t \int_{t_3}^t \int_{t_2}^t r_{14}(t_1, t_2, t_3) \exp\{-h_1(t, t_1) - h_2(t_1, t_2) - h_3(t_2, t_3) \\ - h_4(t_3, 0)\} dt_1 dt_2 dt_3,$$

$$p_{23}(t) = \int_0^t \lambda_{23}(t_2) \exp\{-h_2(t, t_2) - h_3(t_2, 0)\} dt_2,$$

$$p_{24}(t) = \int_0^t \lambda_{24}(t_3) \exp\{-h_2(t, t_3) - h_4(t_3, 0)\} dt_3 + \int_0^t \int_{t_3}^t r_{24}(t_2, t_3) \\ \exp\{-h_2(t, t_2) - h_3(t_2, t_3) - h_4(t_3, 0)\} dt_2 dt_3,$$

$$\text{and } p_{34}(t) = \int_0^t \lambda_{34}(t_3) \exp\{-h_3(t, t_3) - h_4(t_3, 0)\} dt_3.$$

The $\delta_i(t)$ are given by

$$\delta_1(t) = \int_0^t \lambda_{10}(t_4) \exp\{-h_1(t, t_4)\} dt_4 + \sum_{i=1}^3 \int_0^t \int_{t_4}^t \lambda_{i+1,0}(t_4) \lambda_{1,i+1}(t_i) \\ \exp\{-h_1(t, t_1) - h_{i+1}(t_1, t_4)\} dt_1 dt_4$$

$$+ \int_0^t \int_{t_4}^t \int_{t_2}^t \lambda_{30}(t_4) r_{13}(t_1, t_2) \exp\{-h_1(t, t_1) - h_2(t_1, t_2) \\ - h_3(t_2, t_4)\} dt_1 dt_2 dt_4$$

$$+ \int_0^t \int_{t_4}^t \int_{t_3}^t \lambda_{40}(t_4) \lambda_{12}(t_1) \lambda_{24}(t_3) \exp\{-h_1(t, t_1) - h_2(t_1, t_3) \\ - h_4(t_3, t_4)\} dt_1 dt_3 dt_4 + \int_0^t \int_{t_4}^t \int_{t_3}^t \lambda_{40}(t_4) \lambda_{13}(t_2) \lambda_{34}(t_3)$$

$$\exp\{-h_1(t, t_2) - h_3(t_2, t_3) - h_4(t_3, t_4)\} dt_2 dt_3 dt_4$$

$$+\int_0^t \int_{t_4}^t \int_{t_3}^t \int_{t_2}^t \lambda_{40}(t_4) \Gamma_{14}(t_1, t_2, t_3) \exp\{-h_1(t, t_1) - h_2(t_1, t_2) \\ - h_3(t_2, t_3) - h_4(t_3, t_4)\} dt_1 dt_2 dt_3 dt_4.$$

$$\delta_2(t) = \int_0^t \lambda_{20}(t_4) \exp\{-h_2(t, t_4)\} dt_4 + \sum_{i=1}^2 \int_0^t \int_{t_4}^t \lambda_{i+2,0}(t_4) \lambda_{2,i+2}(t_{i+1}) \\ \exp\{-h_2(t, t_{i+1}) - h_{i+2}(t_{i+1}, t_4)\} dt_{i+1} dt_4 \\ + \int_0^t \int_{t_4}^t \int_{t_3}^t \lambda_{40}(t_4) \Gamma_{24}(t_2, t_3) \exp\{-h_2(t, t_2) - h_3(t_2, t_3) \\ - h_4(t_3, t_4)\} dt_2 dt_3 dt_4.$$

$$\delta_3(t) = \int_0^t \lambda_{30}(t_4) \exp\{-h_3(t, t_4)\} dt_4 + \int_0^t \int_{t_4}^t \lambda_{40}(t_4) \lambda_{34}(t_3) \\ \exp\{-h_3(t, t_3) - h_4(t_3, t_4)\} dt_3 dt_4$$

$$\text{and } \delta_4(t) = \int_0^t \lambda_{40}(t_4) \exp\{-h_4(t, t_4)\} dt_4.$$

These expressions for the $p_{ij}(t)$ and the $\delta_j(t)$ illustrate the discussion in Section 3.1.3 for the case $n=4$.

4. SOME APPLICATIONS OF COMPARTMENTAL MODELS TO RELIABILITY

4.1 Introduction

The examples in Section 1.2 indicate the units within the compartments can be interpreted in many ways. Recall these were inulin within a rabbit, people within an organization, beads within a gastrointestinal tract and carcinogenic particles in a mamillary system. In reliability theory, a "unit" may be any part of a system. It need not be basic or undecomposable. It refers only to a component, however complex, whose reliability is of interest to the overall reliability of the system. If a unit begins operation at $t = 0$ and failure occurs at $t = t_0$, then t_0 is said to be the lifetime of that unit. Suppose t_0 is a random variable with distribution function

$$F(t) = \text{Prob } \{t_0 < t\}.$$

The reliability of the unit at time t is the probability of failure free operation in the interval $(0, t)$ and the reliability function is defined to be $R(t) = 1 - F(t)$.

The distribution function is usually assumed to be an intrinsic property of a unit. And all such units are assumed to be homogeneous in the sense that their life lengths are distributed identically. For this to occur the conditions under which "identical" units are used must be homogeneous otherwise their reliabilities would differ due to extrinsic variables.

In this section, the environments in which a set of units function are assumed to be (possibly) heterogeneous. The function $\lambda(t)$ is assumed to reflect the operating environment of a unit at time t , and $\lambda(t)\Delta t$ can be interpreted for small Δt to be the probability that a unit which has functioned without failure up to the instant t will fail in the interval $(t, t+\Delta t)$. More precisely, $\lambda(t)\Delta t+o(\Delta t)$ is the conditional probability of failure at time t given the unit has operated successfully up to that instant.

Letting $R(t, t+\Delta t)$ denote the probability that a unit has functioned without fail during the interval $(t, t+\Delta t)$, it follows that

$$R(t, t+\Delta t) = \frac{R(t+\Delta t)}{R(t)} .$$

Hence the probability of failure during $(t, t+\Delta t)$ is

$$\lambda(t)\Delta t+o(\Delta t) = 1-R(t, t+\Delta t) = \frac{R(t)-R(t+\Delta t)}{R(t)} .$$

Therefore,

$$\lambda(t) = \frac{-R'(t)}{R(t)} ,$$

hence

$$\lambda(t) = \frac{-R'(t)}{R(t)} = \frac{F'(t)}{1-F(t)} \quad (26)$$

provided $F'(t)$ exists and $F(t)<1$.

Solving (26) for $R(t)$ one obtains the reliability function in terms of $\lambda(t)$;

$$R(t) = \exp\{-\int_0^t \lambda(z)dz\}. \quad (27)$$

The function $\lambda(t)$ is of fundamental importance in many fields and is known by a variety of names. In actuarial work it is the "force of decrement" or "force of mortality" and the demographer refers to it as the "age-specific death rate". In vital statistics and extreme value theory it is the "intensity function". In reliability theory $\lambda(t)$ is the hazard or failure rate. Barlow and Prochan [1965] discuss the role of the hazard function in reliability analyses. Barlow et al. [1963] derive many useful properties of $R(t)$ assuming only a monotone hazard function. A listing of system properties using the monotone assumption is found in Prochan [1966].

The interpretation of hazard rate as a conditional probability corresponds exactly to that of transition rate discussed in Section 1, provided "leaving a compartment" is interpreted as failure. Hence, the transition rates $\lambda_{ij}(t)$ can be regarded as hazard rates in a reliability setting and the failure distribution can be found in terms of the hazard rates using equations (26) and (27).

The hazard rate can sometimes be decomposed into constituent parts having particular physical interpretations. An example of this is seen in a competing-risk model where a unit can have several independent modes of failure. The hazard rate for the unit is the sum of the

individual hazards associated with each risk. Such a system is considered in Section 4.3. There are also situations in which the hazard rate cannot be conveniently decomposed but instead the failure distribution is written as a composition of distribution functions. This is called the mixed distribution model and the overall failure is written as a convex sum of failure distributions. Kao [1959] used this device to model the combined failure due to catastrophic failure and wearout failure as a convex sum of two Weibull distributions.

The mixed distribution model allows one to have distinctly different hazard rate functions over different time periods in the life of a device. However, in this model the time domain is still referenced to the moment the unit is turned on.

Mann et al. [1974] discuss the general distribution of time to failure, wherein a unit can fail due to random failure (time-independent) or due to wearout or intrinsic failure (time-dependent). The hazard rate then has the form

$$\lambda(t) = \lambda_{\text{random}} + \lambda_{\text{intrinsic}}(t). \quad (28)$$

In Section 4.2, the hazard functions will be of the form

$$\lambda(t) = \lambda_{\text{random}} + \lambda_{\text{extrinsic}}(t). \quad (29)$$

Unlike the wearout hazard function, the extrinsic or environmental hazard function may be referenced to a time other than the turnon time of the unit. The random hazard may be due to intrinsic or extrinsic

forces and of course has an exponential failure associated with it.

Davis [1952] is a frequently used reference for justifying an assumption of exponential failure for a wide variety of systems.

Some results of Sections 2 and 3 will now be considered in a reliability context. To place these results in perspective, it is necessary briefly to discuss some fundamental system structures and concepts encountered in system reliability analyses. The reliability, $R(t)$, of a system can be increased in many ways but these can be generally classified as either redundancy or repair. The irreversible compartmental model can be thought to represent a redundant system with backup components in a cold standby mode. Hot, warm and cold standbys are differentiated according to the manner in which the standby is loaded. Hot standbys are loaded precisely the same as the operating unit, hence are assumed to fail by the same failure law as the operational unit even though not in use. A warm standby is kept on a reduced load and presumably has a failure rate smaller than an operational or hot standby unit. A cold standby unit is assumed not to lose operational ability while on standby. Furthermore, standbys are considered as being repairable or not repairable. A repairable unit which has failed can be repaired in accordance with some repair time distribution and placed back on standby whereas a non-repairable unit, once it has failed, is lost to all future system function.

Besides these various standby configurations there are the two basic component structures, series and parallel, whose reliability provide lower and upper bounds on $R(t)$ for a fixed number of components (Birnbaum, [1961]). In a series structure all components must operate

for successful system operation, whereas for a parallel structure all but one component can fail and still have system operation.

Gaver [1964] considers two dissimilar units operating redundantly with constant hazard rate and arbitrary repair time distributions and finds the mean time to system failure (MTSF). A more general situation is solved by Gnedenko [1966] where n units are operating in series with only one standby unit. Again, a constant hazard rate is assumed for the operating unit and a general repair time distribution is assumed. In this work, as well as Gaver's, the Laplace transform of the time to failure distribution is found but not inverted. Instead, the transform is used to find the MTSF.

In Gnedenko et al. [1969] a cold standby system with n dissimilar components is discussed and a sequential method for finding $R(t)$ is shown. This is further generalized to allow for failure properly to switch to the standby unit. Varma [1972] uses similar methods and considers n components in series with 2 components in repairable standby. Various repair disciplines are considered with the hazard rates constant and the repair time of standby units assumed to be arbitrary. Kodama [1974] considers a system with two dissimilar units having Erlang-failure distributions and arbitrary repair distributions. Nakagawa and Osaki [1974, 1975] study the stochastic behavior of two dissimilar units assuming both failure and repair are arbitrary functions of time.

4.2 The n-Compartment Catenary System

Consider the n-compartment catenary system illustrated in Figure 12. This can be seen to represent a cold standby redundant system in which the function of system operation is located in one and only one compartment at a given time. Assume the system is functioning in the compartment labeled n at $t = 0$ but has a hazard rate $\lambda_{n-1,n}(t)$ representing the intensity of failure and successful switching to a standby component. The compartment to which the operating function transfers is labeled $n-1$. Assume also that this component can fail in such a way (perhaps a switching failure) that a standby component cannot assume the system function, hence there is system failure. In this case the operating function has transferred to compartment zero.

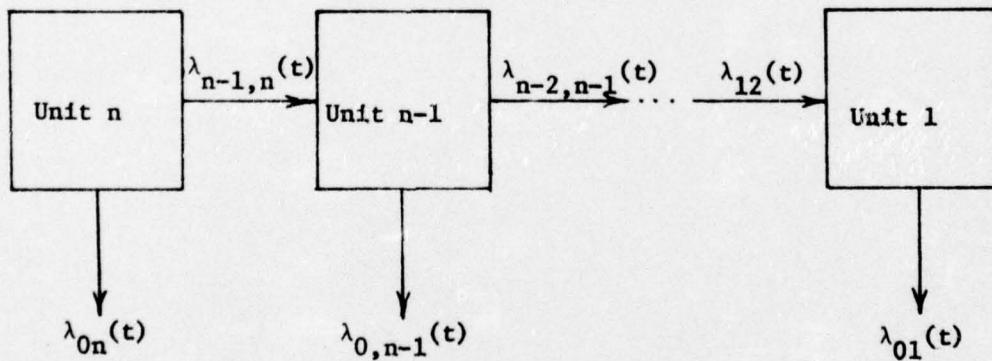


Figure 12
Catenary Model as a Standby Redundant System

The hazard rate for this type of failure is denoted $\lambda_{0n}(t)$. Similar failure interpretations are assumed for the other components.

It is important to remember that the $\lambda_{ij}(t)$ in this compartmental approach have a fundamentally different meaning from those hazard rates normally found in the literature. These differences are seen when one compares equations (28) and (29). Normally hazard rate is considered to be an intrinsic property of a unit which is a function of the time of unit operation. The usual example of this is failure due to wearout. Here the origin is the point in time at which the unit is activated. On the other hand, in the compartmental context, hazard rate is an extrinsic property of a unit determined by the environment in which the unit is operating. For example this may be a heat, altitude or radiation gradient. Now the origin may be the point in time at which the system rather than the standby unit is activated.

In reality, a unit's hazard rate is influenced by both its intrinsic properties and the environmental conditions. If the environmental effect is assumed to be constant, this component of the hazard rate has the "lack of memory" property and is therefore insensitive to the origin of the time scale. In the same way, if the unit's intrinsic effect on the hazard rate is assumed to be constant, this contribution to the unit's reliability is insensitive to the location of the origin. The latter is assumed to be the case in applying this compartmental approach.

4.2.1 The Cumulant Generating Function

Using the cumulant generating function for the mixed model (20) and realizing the $\delta_j(t)$ are identically zero, one can write the cumulant generating function for this catenary system

$$K(\theta, t) = k \left[\ln[1 + e^{\theta_1 - 1} p_{11}(t)], \ln[1 + \sum_{i=1}^2 (e^{\theta_i - 1} p_{i2}(t))], \dots, \right. \\ \left. \ln[1 + \sum_{i=1}^n (e^{\theta_i - 1} p_{in}(t))] \right] \quad (30)$$

where

$$p_{ii}(t) = \exp\{-g_i(t, 0)\}, \quad i = 1, \dots, n,$$

$$p_{li}(t) = \int_0^t \int_{t_{i-1}}^t \dots \int_{t_{l+1}}^t r_{li}(t_l, \dots, t_{i-1}) \exp\{-g_l(t, t_l)\}$$

$$- \sum_{k=l+1}^{i-1} g_k(t_{k-1}, t_k) - g_i(t_{i-1}, 0) \} \prod_{k=l}^{i-1} dt_k,$$

$$i = 2, 3, \dots, n \text{ and } l = 1, 2, \dots, i-1,$$

and

$$g_1(x, y) = \int_y^x \lambda_{01}(z) dz,$$

$$g_i(x, y) = \int_y^x [\lambda_{01}(z) + \lambda_{i-1, i}(z)] dz$$

$$i = 2, 3, \dots, n,$$

and

$$r_{ij}(z_1, \dots, z_{j-1}) = \lambda_{i, i+1}(z_1) \dots \lambda_{j-1, j}(z_{j-1}).$$

However, in the present context this cumulant generating function can be greatly simplified. Recall that an initial distribution of units $x_i(0) = x_i$, for all i , implies

$$k(\theta) = x_1 \theta_1 + \dots + x_n \theta_n. \quad (31)$$

Hence the functional form of k , obtained from (31), can be used in equation (30). Also, since all of the system function is located in compartment n at $t = 0$, the initial distribution is $x_n(t) = x_n$ and $x_i(0) = 0$, $i \neq n$.

Therefore, the cumulant generating function becomes

$$K(\theta, t) = x_n \ln[1 + \sum_{i=1}^n (e^{\theta_i} - 1)p_{in}(t)] \quad (32)$$

where

$$\begin{aligned} p_{in}(t) &= \int_0^t \int_{t_{n-1}}^t \dots \int_{t_{i+1}}^t r_{in}(t_i, \dots, t_{n-1}) \exp\{-g_i(t, t_i)\} \\ &\quad - \sum_{k=i+1}^{n-1} g_k(t_{k-1}, t_k) - g_n(t_{n-1}, 0) \} \prod_{k=1}^{n-1} dt_k \quad i=1, 2, \dots, n-1, \end{aligned}$$

and

$$p_{nn}(t) = \exp\{-g_n(t, 0)\}.$$

4.2.2 The Stochastic Distribution of $(x_1(t), x_2(t), \dots, x_n(t))$

The cumulant generating function in (32) is readily seen to be

associated with an n-variate multinomial distribution with parameters $p_{in}(t)$, $i=1, \dots, n$ and X_n .

Thus the complete distribution of the stochastic vector $(X_1(t), X_2(t), \dots, X_n(t))$ is determined and can be expressed;

$$\text{Prob } \{(X_1(t), X_2(t), \dots, X_n(t))\} =$$

$$\frac{\frac{X_n!}{\prod_{i=1}^n p_{in}(t)^{X_i(t)}} \left[\prod_{i=1}^n p_{in}(t) \right]^{X_n - \sum_{i=1}^n X_i(t)}}{\prod_{i=1}^n X_i(t)! \left[X_n - \sum_{i=1}^n X_i(t) \right]!} \quad (33)$$

where the $p_{in}(t)$ are defined in (32). It follows that the marginals are also multinomials whose parameters can be seen to be sums of appropriate probabilities, $p_{in}(t)$ and X_n .

In particular, the marginal distribution of $X_i(t)$ is binomial with parameters X_n and $p_{in}(t)$. The means, variances and covariances can be written directly from the parameters in (33) or as special cases of the expressions in (21). These are

$$E(X_i(t)) = X_n p_{in}(t),$$

$$V(X_i(t)) = X_n p_{in}(t)(1-p_{in}(t))$$

and

$$\text{cov}(X_i(t), X_j(t)) = -X_n p_{in}(t)p_{jn}(t). \quad (34)$$

Another random variable of particular interest is

$$X_T(t) = \sum_{i=1}^n X_i(t). \quad (35)$$

If one assumes this system is turned on and operated until failure occurs and that this is repeated X_n times, then $X_T(t)$ is the number of repetitions in which the system was still operating at time t .

This variable is clearly distributed as a binomial with parameters

$$X_n \text{ and } \sum_{i=1}^n p_{in}(t). \quad (36)$$

This fact is exploited in the next subsection.

4.2.3 The Probability of Faultless Operation; R(t)

It was assumed that X_n units were placed into operation at time $t = 0$. The expected proportion of these still operating at time t is the reliability. Hence, from (34), (35) and (36)

$$E(X_T(t)) = E\left(\sum_{i=1}^n X_i(t)\right)$$

$$= \sum_{i=1}^n E X_i(t)$$

$$= X_n \sum_{i=1}^n p_{in}(t).$$

Therefore

$$R(t) = E\left[\frac{X_T(t)}{X_n}\right] = \sum_{i=1}^n p_{in}(t), \quad (37)$$

where $p_{in}(t)$ is defined in (32).

An alternative formulation for this application is to consider X_i to be an indicator variable having the value 0 or 1. At time $t = 0$, $X_n = 1$, then $X_i = 1$ provided the system is functioning in compartment i and $X_i = 0$ otherwise. Now the expected value of $X_T(t)$, and hence $R(t)$, will still be given by (37).

4.2.4 Lower Confidence Limit for the System Reliability and the Variance of R(t)

An estimate of $R(t)$ is given by $\hat{R}(t) = \frac{\hat{X}_T(t)}{X_n}$.

Since the distribution of $X_T(t)$ is known to be binomial it is a standard procedure (see Ostle [1972]) to write the lower 100 α per cent confidence limit for $R(t)$ as the smallest value of p satisfying

$$\sum_{i=X_T(t)}^{X_n} \binom{X_n}{i} [p]^i [1-p]^{X_n-i} \geq 1-\alpha. \quad (38)$$

Letting this value be p' one has

$$\text{Prob } \{R(t) \geq p'\} \geq 1-\alpha.$$

The variance of $\hat{R}(t)$ can be derived by considering the variance of $X_T(t)$. That is

$$\text{Var}(X_T(t)) = X_n \sum_{i=1}^n p_{in}(t) \left[1 - \sum_{i=1}^n p_{in}(t) \right].$$

Hence

$$\begin{aligned} \text{Var}(\hat{R}(t)) &= \text{Var}\left[\frac{\bar{X}_T(t)}{X_n}\right] \\ &= \frac{1}{X_n^2} \text{Var}(X_T(t)) \\ &= \frac{1}{X_n} \sum_{i=1}^n p_{in}(t) \left[1 - \sum_{i=1}^n p_{in}(t) \right] \end{aligned} \quad (39)$$

4.2.5 The Mean Time to System Failure (MTSF)

Assuming $f(t)$ is the failure density for the system, then by the definition of expectation,

$$\text{MTSF} = E(t) = \int_0^\infty t f(t) dt. \quad (40)$$

But

$$f(t) = \frac{dR(t)}{dt}$$

so substituting this expression into (40) yields

$$\text{MTSF} = - \int_0^{\infty} t dR(t).$$

Integrating by parts one obtains

$$\text{MTSF} = \int_0^{\infty} R(t) dt. \quad (41)$$

Hence combining (37) and (41) one has

$$\text{MTSF} = \sum_{i=1}^n \int_0^{\infty} p_{in}(t) dt \quad (42)$$

where $p_{in}(t)$, $i=1, 2, \dots, n$ are defined in equation (32).

4.2.6 The Variance of the Lifelength of the System

Using the definition of variance one has

$$\begin{aligned} \text{Var}(t) &= E(t-E(t))^2 \\ &= E(t^2) - [E(t)]^2 \\ &= \int_0^{\infty} t^2 f(t) dt - [E(t)]^2 \end{aligned}$$

$$= 2 \int_0^{\infty} t R(t) dt - [E(t)]^2 \quad (43)$$

Hence from (37), (42) and (43),

$$\text{Var}(t) = 2 \sum_{i=1}^n \int_0^{\infty} t p_{in}(t) dt + \left[\sum_{i=1}^n \int_0^{\infty} p_{in}(t) dt \right]^2 \quad (44)$$

where $p_{in}(t)$ $i=1,2,\dots,n$ are defined in (32).

4.2.7 The Probability Fewer than r units have Failed; $R(r,t)$

Of the X_n units placed into operation at time $t = 0$, the expected proportion of these still operating in compartment $n, n-1, \dots, n-r+1$ is the reliability of the first r units used. This will be denoted $R(r,t)$. Therefore consider

$$\begin{aligned} & E(X_n(t) + X_{n-1}(t) + \dots + X_{n-r+1}(t)) \\ &= E \sum_{i=n-r+1}^n X_i(t) \\ &= X_n \sum_{i=n-r+1}^n p_{in}(t). \end{aligned}$$

Hence

$$R(r,t) = E \left[\frac{\sum_{i=n-r+1}^n X_i(t)}{X_n} \right]$$

$$= \sum_{i=n-r+1}^n p_{in}(t), \quad (45)$$

where the $p_{in}(t)$ are the same as in (32).

Confidence limits on this can be derived in a manner exactly the same as the method used in Subsection 4.2.3.

4.2.8 A Numerical Example Using the Catenary Model

A numerical example will now be considered using a three-compartment system. The joint cumulant generating function is obtained from (32). This is

$$K(\theta, t) = X_3 \ln [1 + \sum_{i=1}^3 (e^{\theta_i} - 1) p_{i3}(t)], \quad (46)$$

where

$$p_{13}(t) = \int_0^t \int_{t_2}^t \lambda_{12}(t_1) \lambda_{23}(t_2) \exp\{-\int_{t_1}^t \lambda_{01}(z) dz - \int_{t_2}^{t_1} [\lambda_{02}(z) + \lambda_{12}(z)] dz$$

$$- \int_0^{t_2} [\lambda_{03}(z) + \lambda_{23}(z)] dz\} dt_1 dt_2,$$

$$p_{23}(t) = \int_0^t \lambda_{23}(t_2) \exp\{-\int_{t_2}^t [\lambda_{02}(z) + \lambda_{12}(z)] dz$$

$$- \int_0^{t_2} [\lambda_{03}(z) + \lambda_{23}(z)] dz\} dt_2$$

and

$$p_{33}(t) = \exp\{-\int_0^t [\lambda_{03}(z) + \lambda_{23}(z)] dz\}.$$

Now let

$$a(t) = \lambda_{12}(t) = \lambda_{23}(t),$$

$$b(t) = \lambda_{02}(t) = \lambda_{03}(t)$$

and

$$a(t)+b(t) = \lambda_{01}(t).$$

This represents a situation in which each unit is vulnerable to two classes of hazards. Those hazards which cause failures for which a standby unit may be provided have hazard function $a(t)$. Those hazards without standby redundancy, such as perhaps hazards to sensing or switching, have hazard function $b(t)$. The last unit to operate is vulnerable to both kinds of failure without standby redundancy.

Now making these substitutions into (46), and assuming

$$A(t) = \int_0^t a(z) dz$$

and

$$B(t) = \int_0^t b(z) dz,$$

one obtains,

$$p_{13}(t) = \int_0^t \int_{t_2}^t a(t_1)a(t_2) \exp\{-\int_0^t [a(z)+b(z)]dz\} dt_1 dt_2,$$

which can be written,

$$p_{13}(t) = \exp\{-A(t)-B(t)\} \frac{[A(t)]^2}{2}.$$

Similarly, one can show

$$p_{23}(t) = \exp\{-A(t)-B(t)\} A(t)$$

and

$$p_{33}(t) = \exp\{-A(t)-B(t)\}.$$

Now the reliability of the system can be obtained from (37).

Therefore

$$\begin{aligned} R(t) &= \sum_{i=1}^3 p_{ii}(t) \\ &= \exp\{-A(t)-B(t)\} \left[1 + A(t) + \frac{[A(t)]^2}{2} \right]. \end{aligned} \quad (47)$$

Now suppose, for further illustration, $a(t)$ is approximately a normal density function (of course a hazard function need not be a probability density function) with a mean of 5 and a variance of 1. Hence $a(0)$ is essentially zero. The other hazard function $b(t)$ will be

taken to be a constant .05. Therefore

$$a(t) = \frac{1}{\sqrt{2\pi}} e^{-(t-5)^2/2}$$

and

$$b(t) = .05.$$

One can now write

$$\begin{aligned} p_{13}(t) &= \exp\{-\Phi(t-5) - .05t\} \frac{[\Phi(t-5)]^2}{2}, \\ p_{23}(t) &= \exp\{-\Phi(t-5) - .05t\} [\Phi(t-5)], \\ p_{33}(t) &= \exp\{-\Phi(t-5) - .05t\}, \end{aligned} \quad (48)$$

where Φ is the cumulative distribution function of a normal (5,1).

Figure 13 shows a graph of the probabilities in (48) and of $R(t)$ given by (47). It is evident that most of the failure in the system occurs from $t = 3$ to $t = 7$ when the $a(t)$ hazard function is dominant. After $t = 7$ the constant hazard function $b(t)$ is causing an exponential failure probability to occur.

The MTSF is obtained from equation (42) where

$$\begin{aligned} \text{MTSF} &= \sum_{i=1}^3 \int_0^\infty p_{i3}(t) dt \\ &= 18.8. \end{aligned}$$

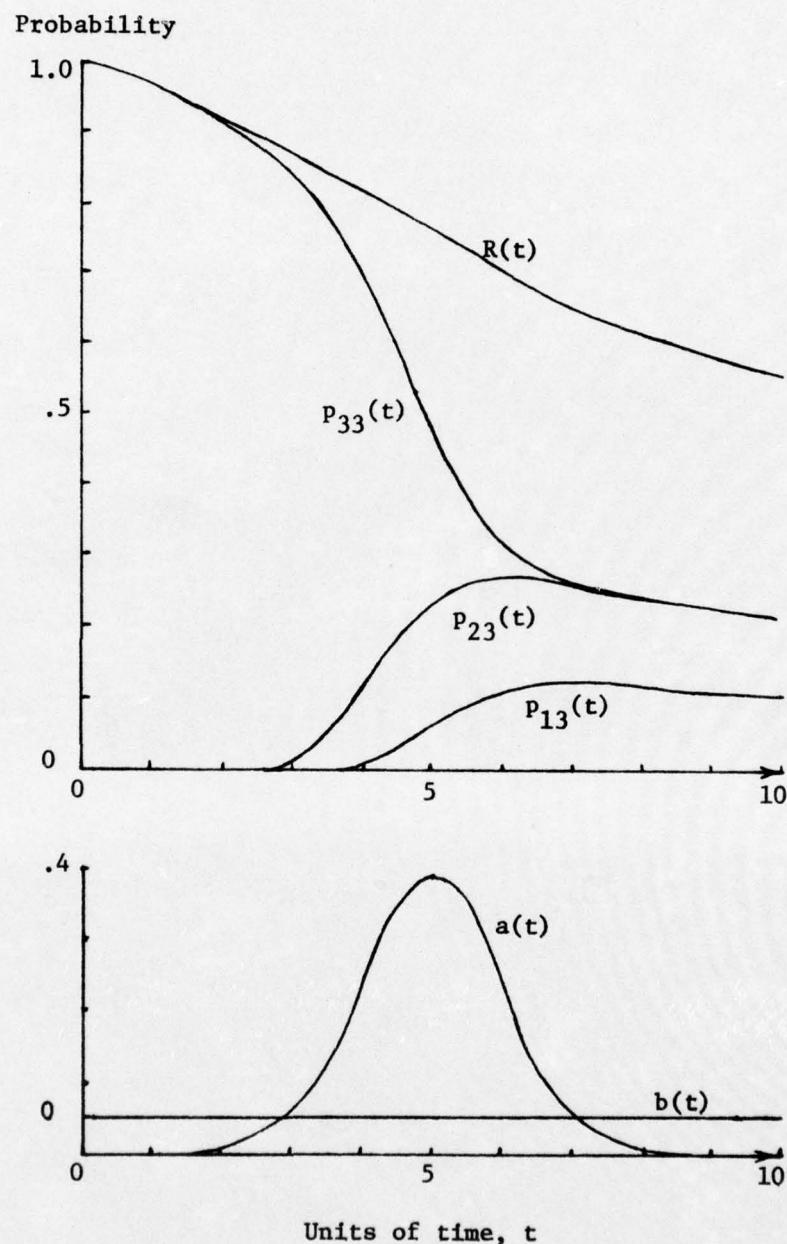


Figure 13

The Probabilities, $p_{ij}(t)$, the System Reliability $R(t)$ and the
hazard Functions $a(t)$ and $b(t)$ for the Catenary Model

The variance of the lifelength is given by equation (44). One obtains

$$\begin{aligned}\text{Var}(t) &= 2 \int_0^{\infty} t R(t) dt - [\text{MTSF}]^2 \\ &= 2(368.79) - (18.80)^2 \\ &= 384.14.\end{aligned}$$

Hence

$$\sqrt{\text{Var}(t)} = 19.60.$$

Using the result in Subsection 4.2.7 one can express the probability fewer than r units have failed, $R(r,t)$. For example, the probability fewer than 2 units have failed is

$$R(2,t) = \sum_{i=2}^3 p_{i3}(t).$$

The expression $R(r,t)$ is simply the reliability of the first r units of the system and many properties can be derived concerning this subsystem by reapplying the results of Section 4.2. The graphs of $R(1,t)$, $R(2,t)$ and $R(t)$ are shown in Figure 14. Also indicated on this figure are the MTSF for the first component, the first and second component and the entire system. The results depicted in Figures 13 and 14 can be found in Table 1.

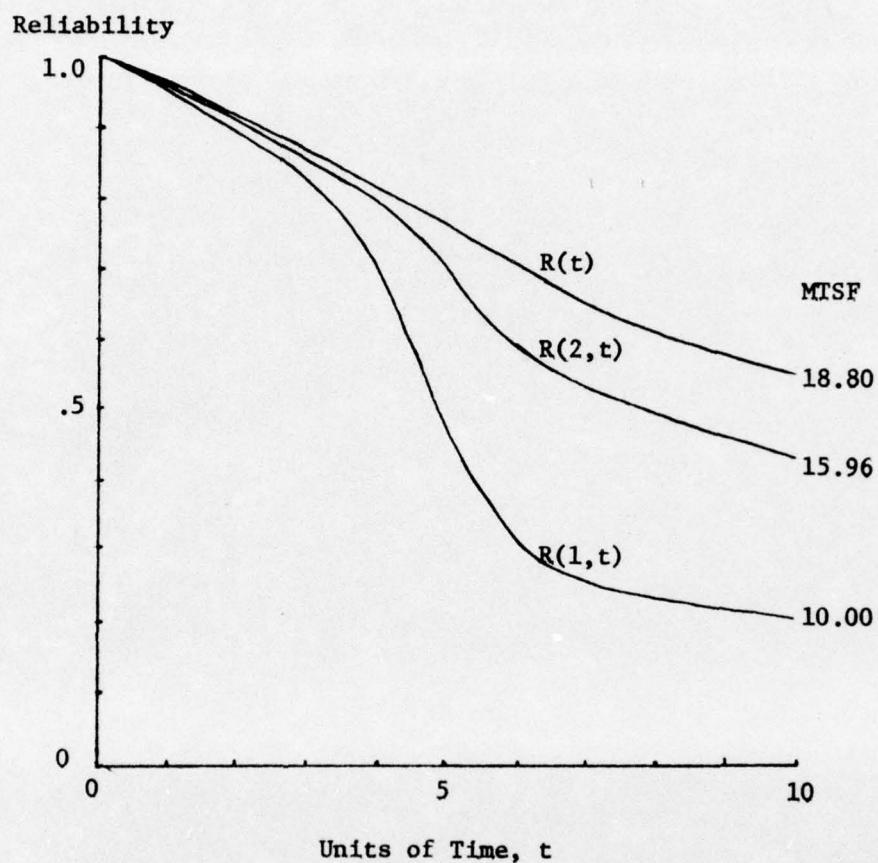


Figure 14

The Reliabilities for One, Two and Three-Compartment Standby Systems

Table 1

Three-Compartment Example of a Standby System Using the Catenary Model

t	$p_{33}(t)$	$p_{23}(t)$	$p_{13}(t)$	$R(1,t)$	$R(2,t)$	$R(t)$
0.0	1.00	0.00	0.00	1.00	1.00	1.00
1.0	0.95	0.00	0.00	0.95	0.95	0.95
2.0	0.90	0.00	0.00	0.90	0.90	0.90
3.0	0.84	0.02	0.00	0.84	0.86	0.86
4.0	0.70	0.11	0.01	0.70	0.81	0.82
5.0	0.47	0.24	0.06	0.47	0.71	0.77
6.0	0.32	0.27	0.11	0.32	0.59	0.70
7.0	0.27	0.26	0.13	0.27	0.53	0.66
8.0	0.25	0.25	0.12	0.25	0.50	0.62
9.0	0.24	0.23	0.12	0.24	0.47	0.59
10.0	0.22	0.22	0.11	0.22	0.44	0.55

4.3 The Mixed Model

Turning now to the general mixed model depicted in Figure 7, this can be interpreted as a Competing-Risk Model with standby redundancy. Mann et al. [1974] give a brief review of the formulation of the Competing-Risk Model and reference researchers who have investigated it. It is assumed that a unit has n modes or risks of failure. One of these has no standby unit and hence may represent a complete failure of the malfunction sensing or switching system. The remaining n-1 risks

have standby units available to provide continuous operation of the system. It is assumed the hazard rate associated with the i^{th} risk at time t is given by $\lambda_{in}(t)$. This time-dependent hazard rate could describe an intrinsic risk to the initial operating unit such as wearout, an extrinsic environmental risk or some combination of the two. However, for subsequent units the risk from intrinsic causes must be assumed constant.

The general solution to this model is given in Section 2.2. Note that the standby units can be assumed to have a further standby structure using the catenary portion of the model. The immigration portion of the model will be assumed to be zero. However, systems themselves could be connected in a probabilistic manner using transfers such as $\lambda_{n0}(t)$.

The three-compartment system depicted in Figure 15 will now be developed in the reliability context. These results can easily be extended to the n -compartment model. In the three-compartment case the initial operating unit can fail in two ways such that standby units are available and one way such that no standby is available and hence system failure occurs. The usual example in which two failures may occur is an electronic device which fails due to an open circuit or due to a short circuit. In general one could have type A, type B or switching failure. It is assumed type B failure can occur to either the initial unit in compartment three or to the standby unit operating in compartment two following a type A failure.

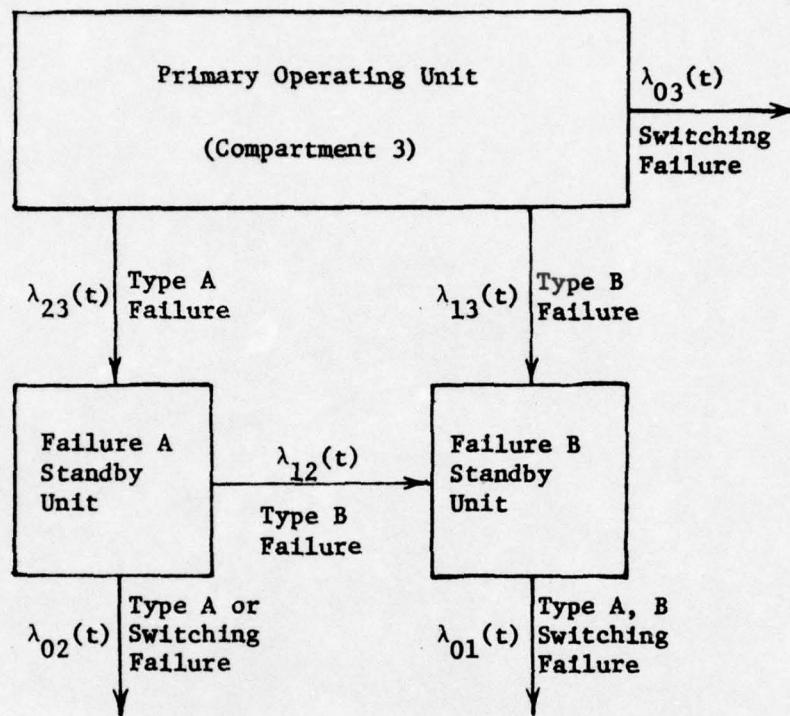


Figure 15

Three-Compartment Competing-Risk Model with Standby Redundancy

4.3.1 The Cumulant Generating Function

Just as in Section 4.2.1, the cumulant generating function can be found from the n-compartment result in equation (20) or by using the three-compartment result given by equation (12). The initial distribution is $X_3(0) = X_3$, $X_1(0) = X_2(0) = 0$, and the $\delta_i(t)$ are identically zero.

Hence,

$$k(\theta_1, \theta_2, \theta_3) = x_3 \theta_3$$

gives the form of the function k .

The cumulant generating function is therefore

$$K(\theta_1, \theta_2, \theta_3, t) = x_3 \ln [1 + \sum_{i=1}^3 (e^{\theta_i} - 1) p_{i3}(t)] \quad (49)$$

where

$$\begin{aligned} p_{13}(t) &= \int_0^t \lambda_{13}(t_2) \exp \left\{ - \int_0^{t_2} (\lambda_{03}(z) + \lambda_{13}(z) + \lambda_{23}(z)) dz - \int_{t_2}^t \lambda_{01}(z) dz \right\} dt_2 \\ &\quad + \int_0^t \int_{t_2}^t \lambda_{12}(t_1) \lambda_{23}(t_2) \exp \left\{ - \int_0^{t_2} (\lambda_{03}(z) + \lambda_{13}(z) + \lambda_{23}(z)) dz \right. \\ &\quad \left. - \int_{t_2}^{t_1} (\lambda_{02}(z) + \lambda_{12}(z)) dz - \int_{t_1}^t \lambda_{01}(z) dz \right\} dt_1 dt_2, \\ p_{23}(t) &= \int_0^t \lambda_{23}(t_2) \exp \left\{ - \int_0^{t_2} (\lambda_{03}(z) + \lambda_{13}(z) + \lambda_{23}(z)) dz \right. \\ &\quad \left. - \int_{t_2}^t (\lambda_{02}(z) + \lambda_{12}(z)) dz \right\} dt_2, \\ p_{33}(t) &= \exp \left\{ - \int_0^t (\lambda_{03}(z) + \lambda_{13}(z) + \lambda_{23}(z)) dz \right\}. \end{aligned}$$

4.3.2 The Stochastic Distribution of $(X_1(t), X_2(t), X_3(t))$

One would expect this vector to have a quadranomial distribution and indeed the cumulant generating function (49) confirms this and provides the parameters X_n , $p_{13}(t)$, $p_{23}(t)$ and $p_{33}(t)$. Thus

$$\text{Prob } \{(X_1(t), X_2(t), X_3(t))\} =$$

$$\frac{\prod_{i=1}^3 \left[p_{13}(t)^{X_1(t)} \right] \left[1 - \sum_{i=1}^3 p_{13}(t) \right]^{X_3 - \sum_{i=1}^3 X_1(t)}}{\prod_{i=1}^3 X_1(t)! \left[X_n - \sum_{i=1}^3 X_1(t) \right]!} \quad (50)$$

where the $p_{ij}(t)$ are defined in (49).

The marginal distributions are completely analogous to the marginals associated with the catenary model discussed in Section 4.2.2. The means, variances and covariances are written as in equation (34). However the parameters are given in (49).

4.3.3 The Probability of Faultless Operation; $R(t)$

Recalling that $X_3(0) = X_3$ and $X_T(t)$ is defined to be

$$X_T(t) = X_1(t) + X_2(t) + X_3(t),$$

the probability of faultless operation up to time t is given by

$$R(t) = E\left[\frac{X_T(t)}{X_3}\right] = p_{13}(t) + p_{23}(t) + p_{33}(t) \quad (51)$$

where the $p_{ij}(t)$, $i=1,2,3$ are defined in (49).

4.3.4 Miscellaneous Properties of Interest

Knowing the complete multivariate distribution of $(X_1(t), X_2(t), X_3(t))$ given in (50), one can derive many interesting properties of the reliability system. Some of these were discussed in detail in Section 4.2 and these derivations will not be repeated now. However, the final expressions are identical in most cases with only the parameters, $p_{ij}(t)$ differing. Thus a discussion of confidence limits can be found in Section 4.2.4. The mean time to system failure and its variance are found in Section 4.2.5 and Section 4.2.6. Other reliability analyses of interest may depend on the particular problem.

4.3.5 A Numerical Example Using the Mixed Model

The three-compartment mixed model illustrated in Figure 15 will be used in this example. The cumulant generating function with the associated parameters $p_{ij}(t)$, $i=1,2,3$ are given by (49). If the hazard functions are assumed to be identical for type A, type B and switching failures then these can be rewritten

$$\begin{aligned}
 a(t) &= \lambda_{23}(t), \\
 b(t) &= \lambda_{12}(t) = \lambda_{13}(t), \\
 c(t) &= \lambda_{03}(t), \\
 a(t) + c(t) &= \lambda_{02}(t), \\
 a(t) + b(t) + c(t) &= \lambda_{01}(t).
 \end{aligned}$$

Suppose also that

$$\begin{aligned}
 A(t) &= \int_0^t a(z)dz, \\
 B(t) &= \int_0^t b(z)dz \\
 \text{and} \quad C(t) &= \int_0^t c(z)dz.
 \end{aligned}$$

Now the parameters in the cumulant generating function can be rewritten

$$\begin{aligned}
 p_{33}(t) &= \exp\{-A(t)-B(t)-C(t)\}, \\
 p_{23}(t) &= \exp\{-A(t)-B(t)-C(t)\}A(t) \\
 \text{and} \quad p_{13}(t) &= \exp\{-A(t)-B(t)-C(t)\} \left[A(t)B(t) - \int_0^t a(z)B(z)dz \right]. \quad (52)
 \end{aligned}$$

Assuming now that $a(t)$ and $b(t)$ are hazards of a periodic nature,

these can be expressed in general as

$$a(t) = a_1 + a_2 \sin(a_3 t + a_4)$$

and

$$b(t) = b_1 + b_2 \sin(b_3 t + b_4).$$

It is easy to show

$$A(t) = a_1 t + \frac{a_2}{a_3} (\cos a_4 - \cos(a_3 t + a_4))$$

and

$$B(t) = b_1 t + \frac{b_2}{b_3} (\cos b_4 - \cos(b_3 t + b_4)).$$

Now keeping $c(t)$ completely general one can write

$$\begin{aligned} p_{33}(t) &= \exp\{-c(t) - (a_1 + b_1)t - \frac{a_2}{a_3}(\cos a_4 - \cos(a_3 t + a_4)) \\ &\quad - \frac{b_2}{b_3}(\cos b_4 - \cos(b_3 t + b_4))\}, \\ p_{23}(t) &= p_{33}(t) [a_1 t + \frac{a_2}{a_3}(\cos a_4 - \cos(a_3 t + a_4))], \\ p_{13}(t) &= p_{33}(t) [(a_1 t + \frac{a_2}{a_3}(\cos a_4 - \cos(a_3 t + a_4)))x \\ &\quad (b_1 t + \frac{b_2}{b_3}(\cos b_4 - \cos(b_3 t + b_4))) - \int_0^t (a_1 + a_2 \sin(a_3 z + a_4))x \\ &\quad (b_1 z + \frac{b_2}{b_3}(\cos b_4 - \cos(b_3 z + b_4))) dz]. \end{aligned} \tag{53}$$

For purposes of this example these expressions will be greatly simplified by assuming $a_1 = b_1 = 1/5$, $i = 1, 2$, $a_3 = b_3 = 1$, $a_4 = 0$ and $b_4 = \pi/2$. In addition let $c(t) \equiv 0$.

The hazard functions are therefore

$$a(t) = \frac{1}{5} + \frac{1}{5} \sin t,$$

$$b(t) = \frac{1}{5} + \frac{1}{5} \cos t,$$

$$c(t) = 0.$$

With these simplified functions, equations (53) become

$$p_{33}(t) = \exp\{(\cos t - \sin t - 2t - 1)/5\},$$

$$p_{23}(t) = p_{33}(t)(t + 1 - \cos t)/5,$$

$$p_{13}(t) = p_{33}(t) \left[\frac{t^2}{2} + \frac{t}{2} - 1 + \cos t + t \sin t - \frac{\sin t \cos t}{2} \right] \frac{1}{25}. \quad (54)$$

These functions are graphed in Figure 16 along with the type A and type B hazard functions. One can note the correspondences between the hazard rates and the probability of being in a particular compartment.

The reliability of the system, $R(t)$, can now be calculated using (51). This function is graphed in Figure 17 and clearly displays the cyclical structure assumed for this model. In addition using

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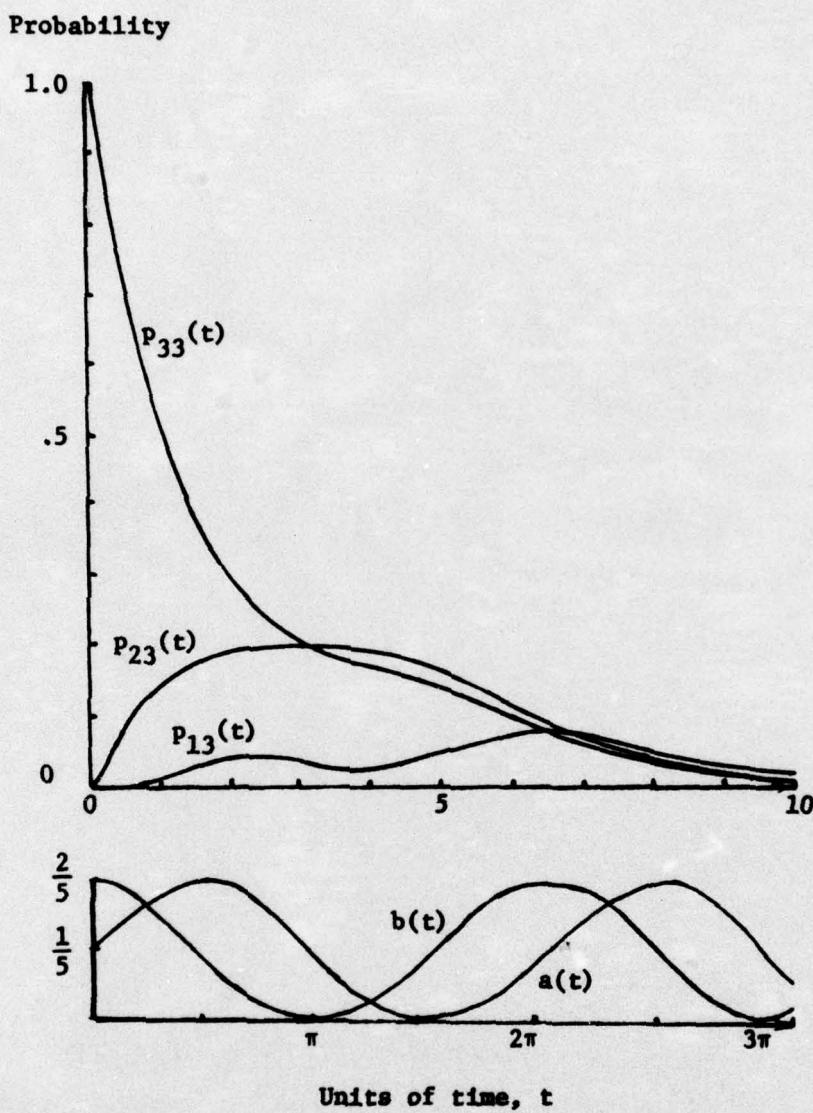


Figure 16

The Probabilities, $p_{ij}(t)$ and the Hazard Functions $a(t)$ and $b(t)$ for
the Mixed Model

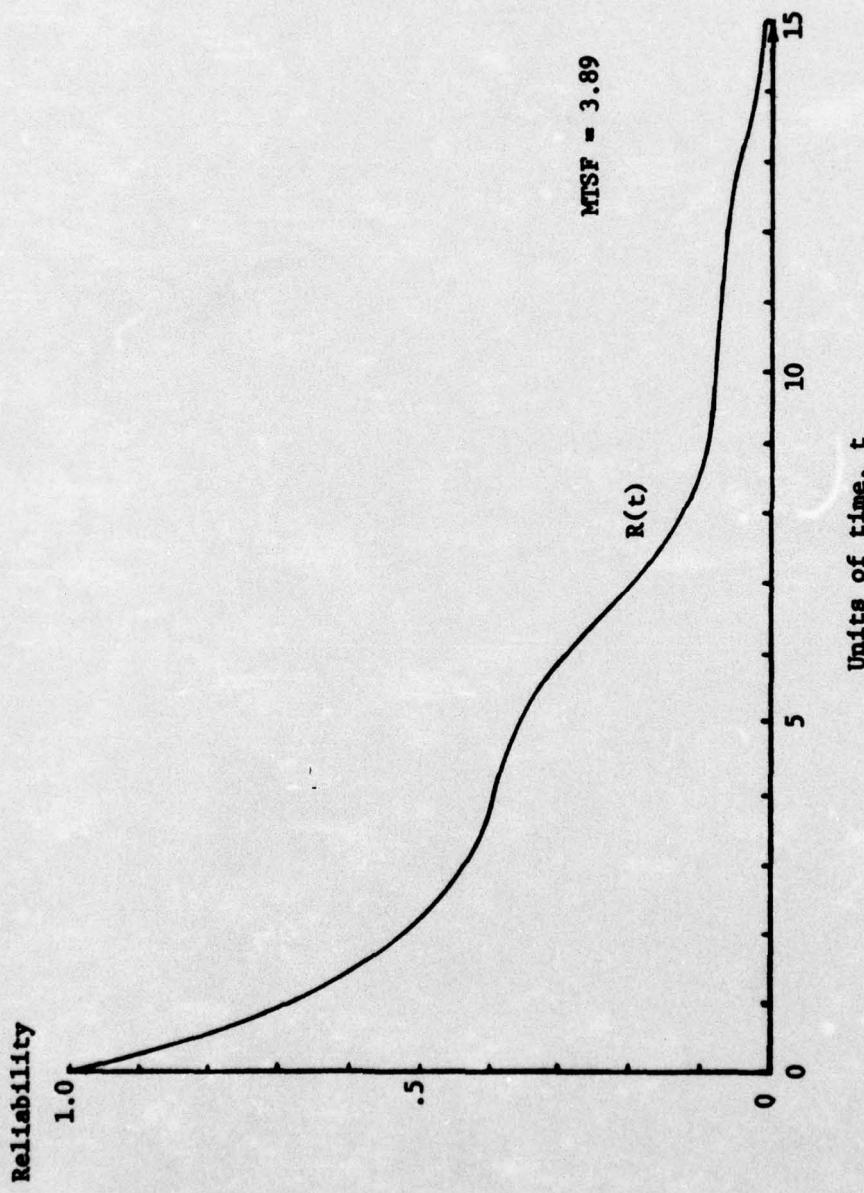


Figure 17

The Reliability of a Three-Compartment Competing-Risk System

$$\text{MTSF} = \int_0^{\infty} R(t)dt$$

one obtains a MTSF of approximately 3.9 units of time. Employing the result given in (43) for the variance of the lifelength of the system one obtains

$$\begin{aligned}\text{Var}(t) &= 2 \int_0^{\infty} t R(t)dt - [E(t)]^2 \\ &= 2 \times 17.48 - (3.89)^2 \\ &= 19.82\end{aligned}$$

The standard deviation of the lifelength is therefore

$$\sqrt{\text{Var}(t)} = 4.45.$$

Table 2 contains the calculated values for $p_{13}(t)$, $p_{23}(t)$, $p_{33}(t)$ and $R(t)$.

Table 2
Three-Compartment Example of a Standby System Using the Mixed Model

t	$p_{33}(t)$	$p_{23}(t)$	$p_{13}(t)$	$R(t)$
0.0	1.0000	0.0000	0.0000	1.0000
1.0	0.5167	0.1509	0.0239	0.6914
2.0	0.2822	0.1928	0.0405	0.5156
3.0	0.1967	0.1963	0.0354	0.4284
4.0	0.1687	0.1908	0.0342	0.3938
5.0	0.1421	0.1624	0.0547	0.3592
6.0	0.0952	0.1150	0.0739	0.2841
7.0	0.0508	0.0736	0.0652	0.1895
8.0	0.0266	0.0486	0.0456	0.1208
9.0	0.0172	0.0375	0.0323	0.0869
10.0	0.0141	0.0335	0.0269	0.0745
11.0	0.0123	0.0295	0.0265	0.0683
12.0	0.0089	0.0216	0.0254	0.0559
13.0	0.0050	0.0130	0.0192	0.0372
14.0	0.0026	0.0076	0.0120	0.0222
15.0	0.0015	0.0051	0.0079	0.0145

4.4 The General Irreversible Model

The use of stochastic compartmental modeling in reliability can be extended to a large class of redundant system structures using the general irreversible model derived in Section 3. Any structure of units or systems of units in which the functional flow is irreversible can be modeled in this way provided the assumptions of Section 4.1 are satisfied.

One can see in Figure 9 there is a hierarchical failure structure in the general model. This structure can be used to evaluate a mission reliability in which certain component failures or malfunctions can only occur in a specific order. For example, in analyzing the reliability of a space craft one could consider an initial class of malfunctions associated with the launch phase. Malfunctions of this kind may be overcome leading eventually to mission success; the malfunction could lead to a problem of another class during a later phase of the mission or mission failure could occur. In a similar manner, if the mission is undergoing a malfunction in a later phase, failure could occur as a consequence; the mission could survive to yet another class of malfunctions or the mission could reach untimate success.

4.4.1 A Numerical Example Using the General Model

In order to illustrate a mission reliability application, a situation will be considered wherein there are three distinct phases of the mission with regard to the type of hazard encountered. These phases are

represented by compartments 1, 2 and 3 in Figure 18.

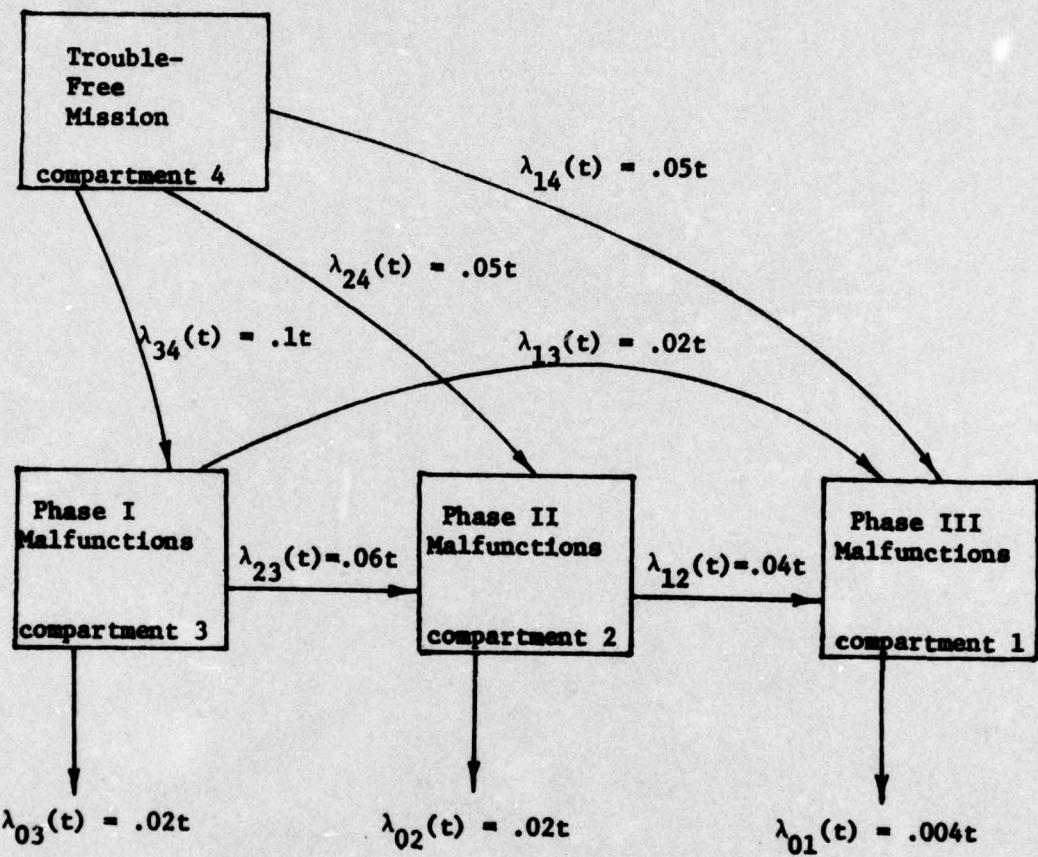


Figure 18

Compartmental Representation of Mission Reliability Example

Compartment 4 represents a trouble-free mission. The only way in which mission failure can occur is through a phase I, II or III malfunction.

The hazard functions in this example were selected primarily for

ease of computation. However they were also selected such that phase I malfunctions are more likely early in the mission and phase II and III malfunctions become more likely as t increases. Also if a phase I malfunction has occurred, then a phase II or phase III malfunction is more likely to occur.

As in the previous examples, the reliability of this mission at time t is given by the probability of being in the compartmental system at time t . This can be determined using the parameters of the cumulant generating function given in Section 3.2. Equation (25) is the cumulant generating function for the four-compartment general irreversible model. Hence using $p_{44}(t)$, $p_{34}(t)$, $p_{24}(t)$ and $p_{14}(t)$ from (25) and the particular hazard rates given in Figure 18, one obtains

$$p_{44}(t) = e^{-0.1t^2},$$

$$p_{34}(t) = e^{-0.05t^2} - e^{-0.1t^2},$$

$$p_{24}(t) = 1.4286 e^{-0.03t^2} + 0.0714 e^{-0.1t^2}$$

$$- 1.5000 e^{-0.05t^2},$$

$$p_{14}(t) = 17.9789 e^{-0.002t^2} - 1.0194 e^{-0.03t^2}$$

$$+ 1.4881 e^{-0.05t^2} - 18.4476 e^{-0.1t^2}.$$

Values for these probabilities have been tabulated in Table 3.

Table 3
Mission Reliability Example Using the General Model

t	$P_{44}(t)$	$P_{34}(t)$	$P_{24}(t)$	$P_{14}(t)$	$R(t)$
0.0	1.0000	0.0000	0.0000	0.0000	1.0000
1.0	0.9048	0.0464	0.0241	0.0242	0.9996
2.0	0.6703	0.1484	0.0868	0.0890	0.9945
3.0	0.4066	0.2311	0.1631	0.1762	0.9769
4.0	0.2019	0.2474	0.2244	0.2690	0.9428
5.0	0.0821	0.2044	0.2509	0.3574	0.8948
6.0	0.0273	0.1380	0.2391	0.4356	0.8400
7.0	0.0074	0.0788	0.1996	0.4995	0.7853
8.0	0.0017	0.0391	0.1484	0.5458	0.7350
9.0	0.0003	0.0171	0.0997	0.5734	0.6905
10.0	0.0000	0.0067	0.0610	0.5835	0.6513
11.0	0.0000	0.0024	0.0343	0.5795	0.6162
12.0	0.0000	0.0007	0.0179	0.5651	0.5837
13.0	0.0000	0.0002	0.0087	0.5438	0.5527
14.0	0.0000	0.0001	0.0039	0.5184	0.5224
15.0	0.0000	0.0000	0.0017	0.4907	0.4923
20.0	0.0000	0.0000	0.0000	0.3466	0.3466
25.0	0.0000	0.0000	0.0000	0.2210	0.2210
30.0	0.0000	0.0000	0.0000	0.1275	0.1275
35.0	0.0000	0.0000	0.0000	0.0666	0.0666
40.0	0.0000	0.0000	0.0000	0.0314	0.0314

In addition, the reliability was calculated using

$$R(t) = \sum_{i=1}^4 p_{14}(t),$$

and these values are included on the table.

Now one can find the mean time to mission failure by applying equation (41). This results in

$$\int_0^\infty R(t)dt = 10.8 \text{ units of time.}$$

The variance of the expected mission length is provided by equation (43). Hence

$$\begin{aligned} \text{Var}(t) &= 2 \int_0^\infty tR(t) - [E(t)]^2 \\ &= 282.56 \end{aligned}$$

and

$$\sqrt{\text{Var}(t)} = 16.8.$$

Similarly, these principles can be applied to the probability of being in the failure-free state at time t , $p_{44}(t)$, to get the mean and variance of the time to first malfunction. Thus

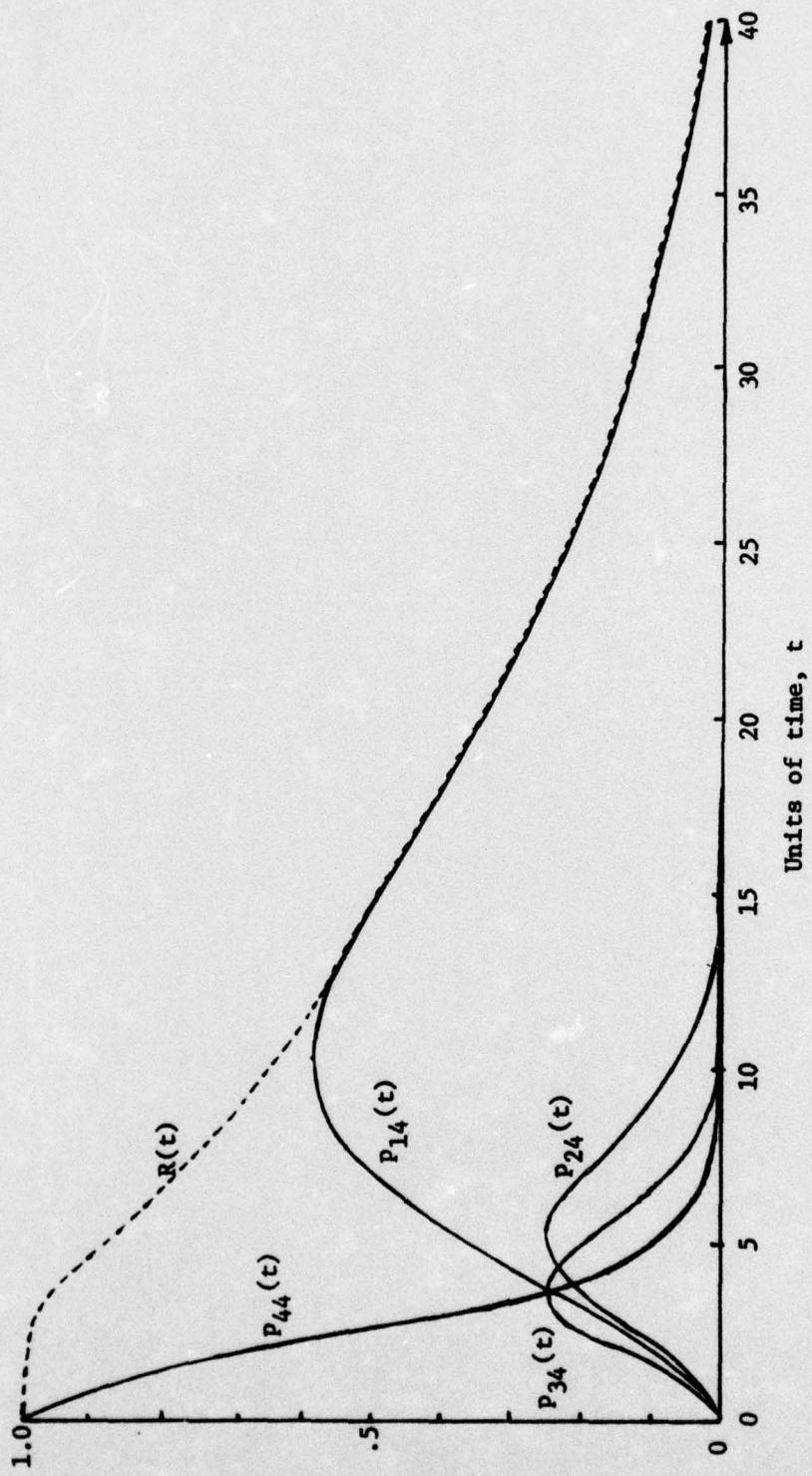
$$\begin{aligned} E(\text{time to first malfunction}) &= \int_0^{\infty} p_{44}(t)dt \\ &= 2.8 \text{ units of time} \end{aligned}$$

and

$$\begin{aligned} \text{Var}(\text{time to first malfunction}) &= 2 \int_0^{\infty} t p_{44}(t)dt - [2.8]^2 \\ &= 2.16. \end{aligned}$$

The values from Table 3 have been graphed in Figure 19. One can see the relatively short time of expected operation without malfunction by the small area under the $p_{44}(t)$ curve.

Also from time 0 to 4, if the system has malfunctioned, it is slightly more likely to be a phase I malfunction, but from time 4 onward the phase III malfunctions become much more likely. Beyond about 15 time units, either the mission has failed or the system is in a phase III malfunction state.



the Reliability of the Mission, $R(t)$

Figure 19

The Probability, $P_{14}(t)$, that a Mission is Malfunction-free or in Malfunction Phase I, II or III, and

5. CONCLUSIONS

5.1 Summary

The cumulant generating functions are derived for a compartmental model which is a mixture of the catenary and mammillary models and a general irreversible model. The first and second moments are found under general assumptions concerning the initial cumulant generating functions and in particular when pulse labeling is assumed the exact multivariate distributions are identified.

Substructures of these models are applied to several reliability situations. A restricted form of the catenary model is used to analyze a standby redundant system. The mixed model is used for a redundant system in which there are multiple risks of component failure. And the general model is used for a mission reliability analysis.

Several fundamental properties of interest in reliability are derived in terms of the hazard rates. Some of these are the system reliability, confidence limits of the reliability, the mean time to system failure and the variance of the lifelength of a system. A numerical example is given of each of these configurations to illustrate some of the concepts developed.

5.2 Future Research

5.2.1 Other Considerations Concerning Reliability

In Section 4, a number of questions arise which are worthy of future study. By what experimental design could one best determine the hazard functions of a given system? It is likely cost would be an important factor in collecting these data, hence optimal designs in terms of time, or equipment would be of interest.

Can one develop a compartmental approach in which the hazard function contains both an age-dependent component and a time-dependent component?

Cardenas and Matis [1974] derive a two-compartment reversible model with time-dependent transition rates. A study should be made to consider the use of this model in reliability where unit repair is considered.

5.2.2 Considerations Concerning Organizational Manpower

The problem of labor turnover has received attention from several researchers and many methods for labor turnover analyses have been proposed. Lane and Andrew [1955] develop a survival curve method wherein a group of new employees are observed until departure from the organization. Inferences are then made based on the type of curve obtained in this way. Herbst [1963] is mentioned in Section 1 with regard to his successful use of a deterministic compartmental approach.

in studying the labor turnover phenomenon. Clowes [1972] simplifies the Herbst model by using fewer compartments. His fit of actual data is still good and his approach is also deterministic. Several other models for social systems can be found in Bartholomew [1973]. More insight into the labor turnover process might be gained by using a stochastic compartmental approach. It would be particularly interesting to use this approach to study the labor turnover process in a graded social structure - such as the military rank system.

5.2.3 Considerations Concerning Survival Distributions

The subject of survival distributions is closely related to the field of reliability. Indeed, one of the most recent works on the subject is by Gross and Clark [1975] who take the approach that theory developed to study the life of a mechanism or a system can in many cases apply just as well to the life of an animal or a human being. There are two concepts developed in Section 4 which could be pursued in the area of survival distributions.

Firstly, the catenary model could be used to model a multistaged disease in which death occurs with differing probability in each stage or transfer to a more advanced stage can occur. Such a model would be particularly well suited in instances where an outside influence affects the transition rate from stage to stage.

An example of this is a seasonal effect or some other periodic influence on the advancement of a disease. The existence of biological rhythms is well established (see Matis et al. [1973]) and the

advancement of some illnesses could be related to these variables using a compartmental model.

Secondly, the mammillary model could be used to investigate competing risks. The theory of competing risks is well advanced (see Chiang [1968]) and it may well be that a stochastic compartmental approach would produce little or no new theory. However, the fact that the compartmental method is different may allow one to obtain previous results in a simpler manner or provide illumination one might not gain otherwise.

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APPENDIX A: DERIVATION OF THE CUMULANT GENERATING FUNCTION
FOR THE GENERAL MODEL

The solution to (22) will now be derived. The subsidiary equations can be written

$$\begin{aligned} \frac{dt}{1} &= \frac{d\theta_1}{(1-e^{-\theta_1})\lambda_{01}(t)} = \frac{d\theta_1}{\sum_{i=1}^{j-1} (1-e^{-\theta_j+\theta_i})\lambda_{ij}(t) + (1-e^{-\theta_j})\lambda_{0j}(t)} \\ &= \frac{dK}{\sum_{j=1}^n (e^{\theta_j-1})\lambda_{j0}(t)}, \quad j = 2, 3, \dots, n. \end{aligned} \tag{A1}$$

Now letting $V_i = (e^{\theta_i}-1)$, $i = 1, 2, \dots, n$, it follows that $dV_i = e^{\theta_i} d\theta_i$. Using this relationship and the subsidiary equations (A1), the following system of ordinary differential equations in the V_i and K can be obtained. This system is

$$\begin{aligned} dV_1 &= V_1 \lambda_{01}(t) dt, \\ dV_i &= \left[\sum_{j=1}^{i-1} (V_i - V_j) \lambda_{ji}(t) + V_i \lambda_{0i}(t) \right] dt, \quad i = 2, 3, \dots, n, \\ dK(\theta, t) &= \sum_{j=1}^n V_j \lambda_{j0}(t) dt. \end{aligned} \tag{A2}$$

Now solving (A2) sequentially for the V_i and $K(\theta, t)$ in terms of the transition rates $\lambda_{ij}(t)$ and $n+1$ constants of integration, this system can be solved for the constants of integration to obtain

$$c_1 = v_1 \exp\{-h_1(t, 0)\},$$

$$c_2 = v_1 \int_0^t \lambda_{12}(t_1) \exp\{-h_1(t, t_1) - h_2(t_1, 0)\} dt_1 + v_2 \exp\{-h_2(t, 0)\},$$

$$c_j = v_1 \left[\int_0^t \lambda_{1j}(t_{j-1}) \exp\{-h_1(t, t_{j-1}) - h_j(t_{j-1}, 0)\} dt_{j-1} \right.$$

$$+ \sum_{k=2}^{j-1} \int_0^t \int_{t_{j-1}}^t \lambda_{1k}(t_{k-1}) \lambda_{kj}(t_{j-1}) \exp\{-h_1(t, t_{k-1})$$

$$- h_k(t_{k-1}, t_{j-1}) - h_j(t_{j-1}, 0)\} dt_{k-1} dt_{j-1} + \dots$$

$$+ \sum_{1 < k_1 < k_2 < \dots < j} \int_0^t \int_{t_{j-1}}^t \dots \int_{t_{k_2-1}}^t \lambda_{kk_1}(t_{k_1-1})$$

$$\prod_{i=1}^{m-2} (\lambda_{k_1, k_{i+1}}(t_{k_{i+1}-1})) \lambda_{k_{m-1}, j}(t_{j-1}) \exp\{-h_1(t, t_{k_1-1})$$

$$- \sum_{i=1}^{m-2} h_{k_1}(t_{k_1-1}, t_{k_{i+1}-1}) - h_j(t_{j-1}, 0) \prod_{i=1}^{m-1} dt_{k_1-1} dt_{j-1} + \dots$$

$$+ \int_0^t \int_{t_{j-1}}^t \dots \int_{t_{k+1}}^t r_{1j}(t_1, t_2, \dots, t_{j-1}) \exp\{-h_1(t, t_1)$$

$$- \sum_{k=2}^{j-1} h_k(t_{k-1}, t_k) - h_j(t_{j-1}, 0) \prod_{k=1}^{j-1} dt_k \Big]$$

$$+ \sum_{i=2}^{j-2} v_1 \left[\int_0^t \lambda_{1j}(t_{j-1}) \exp\{-h_1(t, t_{j-1}) - h_j(t_{j-1}, 0)\} dt_{j-1} \right.$$

$$+ \sum_{k=i+1}^{j-1} \int_0^t \int_{t_{j-1}}^t \lambda_{1k}(t_{k-1}) \lambda_{kj}(t_{j-1}) \exp\{-h_1(t, t_{k-1})$$

$$- h_k(t_{k-1}, t_{j-1}) - h_j(t_{j-1}, 0)\} dt_{k-1} dt_{j-1} + \dots$$

$$\begin{aligned}
& + \sum_{1 < \ell_1 < \ell_2 < \dots < \ell_{m-1} < j} \int_0^t \int_{t_{j-1}}^t \dots \int_{t_{\ell_2-1}}^t \lambda_{1\ell_1}(t_{\ell_1-1}) \\
& \quad \prod_{i=1}^{m-2} (\lambda_{\ell_i, \ell_{i+1}}(t_{\ell_{i+1}-1})) \lambda_{\ell_{m-1}, j}(t_{j-1}) \exp\{-h_1(t, t_{\ell_1-1})\} \\
& - \sum_{i=1}^{m-2} h_{\ell_i}(t_{\ell_i-1}, t_{\ell_{i+1}-1}) - h_j(t_{j-1}, 0) \prod_{i=1}^{m-1} dt_{\ell_i-1} dt_{j-1} + \dots \\
& + \int_0^t \int_{t_{j-1}}^t \dots \int_{t_{\ell_1+1}}^t r_{ij}(t_i, t_{i+1}, \dots, t_{j-1}) \exp\{-h_1(t, t_i)\} \\
& - \sum_{\ell=i+1}^{j-1} h_\ell(t_{\ell-1}, t_\ell) - h_j(t_{j-1}, 0) \prod_{\ell=1}^{j-1} dt_\ell \Big] \\
& + v_{j-1} \int_0^t \lambda_{j-1, j}(t_{j-1}) \exp\{-h_{j-1}(t, t_{j-1}) - h_j(t_{j-1}, 0)\} dt_{j-1} \\
& + v_j \exp\{-h_j(t, 0)\}, \quad j = 3, 4, \dots, n,
\end{aligned}$$

and

$$\begin{aligned}
c_{n+1} &= K(\underline{0}, t) - v_1 \left[\int_0^t \lambda_{10}(t_n) \exp\{-h_1(t, t_n)\} dt_n \right. \\
& + \sum_{i=2}^n \int_0^t \int_{t_n}^t \lambda_{10}(t_n) \lambda_{1i}(t_{i-1}) \exp\{-h_1(t, t_{i-1}) \right. \\
& \quad \left. \left. - h_i(t_{i-1}, t_n)\right) dt_{i-1} dt_n \right. \\
& + \sum_{k=2}^{n-1} \sum_{\ell=2}^k \int_0^t \int_{t_n}^t \int_{t_\ell}^t \lambda_{k+1, 0}(t_n) \lambda_{1k}(t_{k-1}) \lambda_{k, \ell+1}(t_\ell) \\
& \quad \exp\{-h_1(t, t_{k-1}) - h_k(t_{k-1}, t_\ell) - h_{\ell+1}(t_\ell, t_n)\} dt_{k-1} dt_\ell dt_n + \dots \\
& + \sum_{1 < \ell_1 < \ell_2 < \dots < \ell_{m-1} < n} \int_0^t \int_{t_n}^t \int_{t_{\ell_{m-1}-1}}^t \dots \int_{t_{\ell_2-1}}^t \lambda_{k-1, 0}(t_n)
\end{aligned}$$

$$\begin{aligned}
& \lambda_{j, k_1}(t_{k_1-1}) \prod_{i=1}^{m-2} \lambda_{k_i, k_{i+1}}(t_{k_{i+1}-1}) \exp(-h_1(t, t_{k_1-1})) \\
& - \sum_{i=1}^{m-2} h_{k_i}(t_{k_i-1}, t_{k_{i+1}-1}) - h_{k_{m-1}}(t_{k_{m-1}-1}, t_n) \} \prod_{i=1}^{m-1} dt_{k_i-1} dt_n + \dots \\
& + \int_0^t \int_{t_n}^t \dots \int_{t_2}^t \lambda_{n0}(t_n) r_{1n}(t_1, t_2, \dots, t_{n-1}) \\
& \left. \exp\{-h_1(t, t_1) - \sum_{i=1}^{n-1} h_{i+1}(t_i, t_{i+1})\} \prod_{i=1}^n dt_i \right] - \dots \\
& - v_{n-2} \left[\int_0^t \lambda_{n-2, 0}(t_n) \exp\{-h_{n-2}(t, t_n)\} dt_n \right. \\
& + \int_0^t \int_{t_n}^t \lambda_{n-1, 0}(t_n) \lambda_{n-2, n-1}(t_{n-2}) \exp\{-h_{n-2}(t, t_{n-2}) \\
& - h_{n-1}(t_{n-2}, t_n)\} dt_{n-2} dt_n + \int_0^t \int_{t_n}^t \lambda_{n0}(t_n) \lambda_{n-2, n}(t_{n-1}) \\
& \exp\{-h_{n-2}(t, t_{n-1}) - h_n(t_{n-1}, t_n)\} dt_{n-1} dt_n \\
& + \int_0^t \int_{t_n}^t \int_{t_{n-1}}^t \lambda_{n0}(t_n) \lambda_{n-2, n-1}(t_{n-2}) \lambda_{n-1, n}(t_{n-1}) \\
& \exp\{-h_{n-2}(t, t_{n-2}) - h_{n-1}(t_{n-2}, t_{n-1}) - h_n(t_{n-1}, t_n)\} \\
& \left. dt_{n-2} dt_{n-1} dt_n \right] \\
& - v_{n-1}(t) \left[\int_0^t \lambda_{n-1, 0}(t_n) \exp\{-h_{n-1}(t, t_n)\} dt_n \right. \\
& + \int_0^t \int_{t_n}^t \lambda_{n0}(t_n) \lambda_{n-1, n}(t_{n-1}) \exp\{-h_{n-1}(t, t_{n-1}) \\
& - h_n(t_{n-1}, t_n)\} dt_{n-1} dt_n \left. \right]
\end{aligned}$$

$$= v_n \int_0^t \lambda_{n0}(t_n) \exp\{-h_n(t, t_n)\} dt_n \quad (A3)$$

where

$$h_i(x, y) = \int_y^x \sum_{j=0}^{i-1} \lambda_{ji}(z) dz$$

and

$$\Gamma_{ij}(z_1, \dots, z_{j-1}) = \lambda_{i,i+1}(z_1) \dots \lambda_{j-1,j}(z_{j-1}).$$

Now substitute back $e^{\theta_i - 1}$ for v_i and let $c_i = u_i(\theta, t)$ and

$$p_{ii}(t) = \exp\{-h_i(t, 0)\}, \quad i = 1, 2, \dots, n,$$

$$p_{i,i+1}(t) = \int_0^t \lambda_{i,i+1}(t_i) \exp\{-h_i(t, t_i) - h_{i+1}(t_i, 0)\} dt_i, \quad i=1, 2, \dots, n-1,$$

$$p_{ij}(t) = \int_0^t \lambda_{ij}(t_{j-1}) \exp\{-h_i(t, t_{j-1}) - h_j(t_{j-1}, 0)\} dt_{j-1}$$

$$+ \sum_{l=i+1}^{j-1} \int_0^t \int_{t_{j-1}}^t \lambda_{il}(t_{l-1}) \lambda_{lj}(t_{j-1}) \exp\{-h_i(t, t_{l-1})$$

$$- h_l(t_{l-1}, t_{j-1}) - h_j(t_{j-1}, 0)\} dt_{l-1} dt_{j-1} + \dots$$

$$+ \sum_{i < l_1 < l_2 < \dots < l_{m-1} < j} \int_0^t \int_{t_{j-1}}^t \dots \int_{t_{l_2-1}}^t \lambda_{il_1}(t_{l_1-1})$$

$$\prod_{i=1}^{m-2} (\lambda_{l_i, l_{i+1}}(t_{l_{i+1}-1})) \lambda_{l_{m-1}, j}(t_{j-1}) \exp\{-h_i(t, t_{l_1-1})\}$$

$$- \sum_{i=1}^{m-2} h_{l_i}(t_{l_i-1}, t_{l_{i+1}-1}) - h_j(t_{j-1}, 0) \prod_{i=1}^{m-1} dt_{l_i-1} dt_{j-1} + \dots$$

$$+ \int_0^t \int_{t_{j-1}}^t \dots \int_{t_{l+1}}^t \Gamma_{ij}(t_i, t_{i+1}, \dots, t_{j-1}) \exp\{-h_i(t, t_i)\}$$

$$- \sum_{k=i+1}^{j-1} h_k(t_{k-1}, t_k) - h_j(t_{j-1}, 0) \prod_{l=1}^{j-1} dt_l \Big],$$

$j=3, 4, \dots, n$ and $i=1, \dots, j-2$,

$$\delta_n(t) = \int_0^t \lambda_{n0}(t_n) \exp\{-h_n(t, t_n)\} dt_n,$$

$$\delta_{n-1}(t) = \int_0^t \lambda_{n-1,0}(t_n) \exp\{-h_{n-1}(t, t_n)\} dt_n + \int_0^t \int_{t_n}^t \lambda_{n0}(t_n) \lambda_{n-1,n}(t_{n-1})$$

$$\exp\{-h_{n-1}(t, t_{n-1}) - h_n(t_{n-1}, t_n)\} dt_{n-1} dt_n,$$

$$\delta_{n-2}(t) = \int_0^t \lambda_{n-2,0}(t_n) \exp\{-h_{n-2}(t, t_n)\} dt_n$$

$$+ \int_0^t \int_{t_n}^t \lambda_{n-1,0}(t_n) \lambda_{n-2,n-1}(t_{n-2}) \exp\{-h_{n-2}(t, t_{n-2})$$

$$- h_{n-1}(t_{n-2}, t_n)\} dt_{n-2} dt_n + \int_0^t \int_{t_n}^t \lambda_{n0}(t_n) \lambda_{n-2,n}(t_{n-1})$$

$$\exp\{-h_{n-2}(t, t_{n-1}) - h_n(t_{n-1}, t_n)\} dt_{n-1} dt_n$$

$$+ \int_0^t \int_{t_n}^t \int_{t_{n-1}}^t \lambda_{n0}(t_n) \lambda_{n-2,n-1}(t_{n-2}) \lambda_{n-1,n}(t_{n-1})$$

$$\exp\{-h_{n-2}(t, t_{n-2}) - h_{n-1}(t_{n-2}, t_{n-1}) - h_n(t_{n-1}, t_n)\} dt_{n-2} dt_{n-1} dt_n$$

and in general

$$\delta_j(t) = \int_0^t \lambda_{j0}(t_n) \exp\{-h_j(t, t_n)\} dt_n + \sum_{i=j+1}^n \int_0^t \int_{t_n}^t \lambda_{i0}(t_n) \lambda_{ji}(t_{i-1})$$

$$\exp\{-h_j(t, t_{i-1}) - h_i(t_{i-1}, t_n)\} dt_{i-1} dt_n$$

$$\begin{aligned}
& + \sum_{k=2}^{n-j} \sum_{l=j+1}^{j+k-1} \int_0^t \int_{t_n}^t \int_{t_{j+l-1}}^t \lambda_{j+l,0}(t_n) \lambda_{j,k}(t_{k-1}) \lambda_{k,j+l}(t_{j+l-1}) \\
& \exp \{-h_j(t, t_{k-1}) - h_k(t_{k-1}, t_{j+l-1}) - h_{j+l}(t_{j+l-1}, t_n)\} \\
& \quad dt_{k-1} dt_{j+l-1} dt_n + \dots \\
& + \sum_{j < \ell_1 < \ell_2 < \dots < \ell_{m-1}} \int_0^t \int_{t_n}^t \int_{t_{\ell_{m-1}-1}}^t \dots \int_{t_{\ell_2-1}}^t \lambda_{\ell_{m-1},0}(t_n) \lambda_{j,\ell_1}(t_{\ell_1-1}) \\
& \prod_{i=1}^{m-2} \lambda_{\ell_1, \ell_{i+1}}(t_{\ell_{i+1}-1}) \exp \{-h_j(t, t_{\ell_1-1}) - \sum_{i=1}^{m-2} h_{\ell_i}(t_{\ell_i-1}, t_{\ell_{i+1}-1}) \\
& - h_{\ell_{m-1}}(t_{\ell_{m-1}-1}, t_n) \} \prod_{i=1}^{m-1} dt_{\ell_i-1} dt_n + \dots \\
& + \int_0^t \int_{t_n}^t \dots \int_{t_{j+2}}^t \int_{t_{j+1}}^t \lambda_{n0}(t_n) \Gamma_{jn}(t_j, t_{j+1}, \dots, t_{n-1}) \\
& \exp \{-h_j(t, t_j) - \sum_{i=j}^{n-1} h_{i+1}(t_i, t_{i+1})\} \prod_{i=j}^n dt_i. \tag{A4}
\end{aligned}$$

Now (A3) can be written more concisely as

$$\begin{aligned}
c_1 & = u_1(\underline{\theta}, t) = (e^{\theta_1} - 1) p_{11}(t), \\
c_2 & = u_2(\underline{\theta}, t) = (e^{\theta_1} - 1) p_{12}(t) + (e^{\theta_2} - 1) p_{22}(t), \\
& \vdots \\
c_j & = u_j(\underline{\theta}, t) = \sum_{i=1}^j (e^{\theta_{i-1}} - 1) p_{ij}(t), \\
& \vdots \\
c_{n+1} & = u_{n+1}(\underline{\theta}, t) = K(\underline{\theta}, t) - \sum_{j=1}^n (e^{\theta_{j-1}} - 1) \delta_j(t) \tag{A5}
\end{aligned}$$

where the $p_{ij}(t)$ and $\delta_j(t)$ are given by (A4).

By characteristic theory, these $n+1$ constants can be related by a functional relationship ψ such that

$$u_{n+1}(\theta, t) = \psi(u(\theta, t)). \quad (A6)$$

The form of ψ will be determined by the initial conditions. When $t = 0$ the functions u_i become

$$u_i(\theta, 0) = e^{\theta_i - 1} \quad i=1, 2, \dots, n$$

and

$$u_{n+1}(\theta, 0) = K(\theta, 0) = k(\theta).$$

Hence when $t = 0$, equation (A6) reduces to

$$k(\theta) = \psi(e^{\theta_1 - 1}, e^{\theta_2 - 1}, \dots, e^{\theta_n - 1}). \quad (A7)$$

In order to write ψ in the usual functional form let $y_1 = e^{\theta_1 - 1}$. This implies that $\theta_1 = \ln(y_1 + 1)$ and (A7) now becomes

$$k(\ln(y_1 + 1), \dots, \ln(y_n + 1)) = \psi(y_1, y_2, \dots, y_n). \quad (A8)$$

The function ψ has now been defined by the initial form of the joint cumulant generating function. Therefore from equations (A6) and (A8)

$$u_{n+1}(\underline{\theta}, t) = k(\ln(u_1(\underline{\theta}, t)+1), \dots, \ln(u_n(\underline{\theta}, t)+1)). \quad (A9)$$

The solution to (22) can now be obtained by substituting (A5) into (A9) to obtain (23).

APPENDIX B: DERIVATION OF THE MOMENTS FOR THE MIXED MODEL
AND GENERAL MODEL

The moments will be derived by differentiating (20) or (23) with respect to the appropriate parameters and evaluating this for $\theta_i = 0$ $i = 1, \dots, n$. Define

$$u_j = \ln[1 + \sum_{i=1}^j (e^{\theta_i} - 1) p_{ij}(t)] \quad \text{for } j = 1, 2, \dots, n.$$

Therefore (20) can be written

$$K(\theta, t) = k(u) + \sum_{j=1}^n (e^{\theta_j} - 1) \delta_j(t) \quad (B1)$$

Hence

$$\frac{\partial K(\theta, t)}{\partial \theta_i} = \sum_{k=1}^n \left(\frac{\partial k(u)}{\partial u_k} \frac{\partial u_k}{\partial \theta_i} \right) + e^{\theta_i} \delta_i(t) \quad \text{for } i = 1, 2, \dots, n. \quad (B2)$$

The second partial derivative of (B1) with respect to θ_i is

$$\begin{aligned} \frac{\partial^2 K(\theta, t)}{\partial \theta_i^2} &= \sum_{k=1}^n \left\{ \left[\sum_{l=1}^n \frac{\partial^2 k(u)}{\partial u_k \partial u_l} \frac{\partial u_l}{\partial \theta_i} \right] \frac{\partial u_k}{\partial \theta_i} \right. \\ &\quad \left. + \frac{\partial^2 u_k}{\partial \theta_i^2} \frac{\partial k(u)}{\partial u_k} \right\} + e^{\theta_i} \delta_i(t) \quad \text{for } i = 1, 2, \dots, n \end{aligned} \quad (B3)$$

And the partial derivative of (B2) with respect to θ_j is

$$\frac{\partial^2 K(\theta, t)}{\partial \theta_j \partial \theta_i} = \sum_{k=1}^n \left\{ \left[\sum_{l=1}^n \frac{\partial^2 k(u)}{\partial u_l \partial u_k} \frac{\partial u_l}{\partial \theta_j} \right] \frac{\partial u_k}{\partial \theta_i} + \frac{\partial k(u)}{\partial u_k} \frac{\partial^2 u_k}{\partial \theta_j \partial \theta_i} \right\} \quad i, j = 1, \dots, n, \quad i \neq j. \quad (B4)$$

Now consider

$$\frac{\partial u_1}{\partial \theta_1} = \frac{e^{\theta_1} p_{1j}(t)}{1 + \sum_{i=1}^j (e^{\theta_1} - 1) p_{1j}(t)}.$$

Hence

$$\frac{\partial u_1}{\partial \theta_1} \Bigg|_{\text{All } \theta's = 0} = \begin{cases} p_{1j}(t) & i \leq j \\ 0 & i > j. \end{cases} \quad (B5)$$

Also

$$\frac{\partial^2 u_1}{\partial \theta_1^2} = \frac{[1 + \sum_{i=1}^j (e^{\theta_1} - 1) p_{1j}(t)] \cdot e^{\theta_1} p_{1j}(t) - [e^{\theta_1} p_{1j}(t)]^2}{[1 + \sum_{i=1}^j (e^{\theta_1} - 1) p_{1j}(t)]^2}.$$

Therefore

$$\frac{\partial^2 u_1}{\partial \theta_1^2} \Bigg|_{\text{All } \theta's = 0} = \begin{cases} p_{1j}(t) - p_{1j}^2(t) & i \leq j \\ 0 & i > j. \end{cases} \quad (B6)$$

Similarly one obtains

$$\left. \frac{\partial^2 u_k}{\partial \theta_j \partial \theta_1} \right|_{\text{All } \theta's = 0} = \begin{cases} -p_{ik}(t)p_{jk}(t) & i, j \leq k, i \neq j \\ 0 & i \text{ or } j > k. \end{cases} \quad (B7)$$

Assuming the means, variances and covariances for the initial distribution are as defined in Subsections 2.1.3, 2.2.3 and 3.1.4, one can combine (B2), (B3) and (B4) with (B5), (B6) and (B7) to obtain the expressions for $E(X_i(t))$, $V(X_i(t))$ and $\text{cov}(X_i(t), X_j(t))$ as shown in (21) and (24).

VITA

Jon Ohman Epperson was born in Alva, Oklahoma, September 16, 1937. He is the son of Reverend Mitchell Stokes Epperson and Mrs. Esther Rooker Epperson. Mrs. Epperson, now widowed, lives in Corrales, New Mexico. Her mailing address, and permanent address for Jon Epperson, is P.O. Box 574, Corrales, New Mexico, 87048.

Before Jon was one year old, Mr. Epperson was called to the First Presbyterian Church in Ada, Oklahoma where Jon attended public school until the age of 12. In January, 1949, the Eppersons moved to Albuquerque, New Mexico and Jon graduated from Albuquerque High School in 1956. For two years Jon attended The College of Wooster at Wooster, Ohio, then transferred to the University of New Mexico at Albuquerque where he completed a Bachelor of Science degree, with a major in mathematics, in January, 1962.

Jon entered the U.S. Air Force in March, 1962 and has since been stationed at Little Rock, Arkansas; Columbia, Missouri; Washington, D.C.; Colorado Springs, Colorado and College Station, Texas. At the University of Missouri, he completed a Master of Arts degree in mathematics in January, 1968. After three and a half years at the Pentagon and two on the mathematics faculty at the U.S. Air Force Academy, Jon came to Texas A&M University to seek a Doctor of Philosophy degree in the Institute of Statistics. He expects to complete this degree by August, 1976 and then return to the mathematics department at the Air Force Academy.

The typist for this dissertation was Mrs. Susan Epperson.